On Some Statistical Challenges Coming with Non-Euclidean Data

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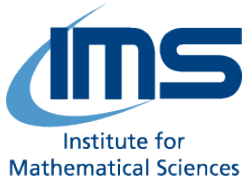
Workshop and Tutorial on High Dimensional Data Analysis



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Outline

Euclidean SLLN and CLT

Let $X_1, \ldots, X_n \overset{\text{i.i.d.}}{\sim} X \in \mathbb{R}^m$, $m \in \mathbb{N}$, and $\bar{X}_n = \frac{1}{n}\sum_{j=1}^{n} X_j$

Theorem (Strong Law of Large Numbers)

$$E[\|X\|] < \infty \Rightarrow \bar{X}_n \overset{a.s.}{\to} \mathbb{E}[X]$$

Theorem (Central Limit Theorem)

$$E[\|X\|^2] < \infty \Rightarrow \sqrt{n}(\bar{X}_n - \mathbb{E}[X]) \overset{\mathbb{P}}{\to} \mathcal{N}(0, \text{cov}[X])$$

Euclidean PCA

Spectral decomposition giving main modes of variation

- $\mathrm{cov}[X] = \Gamma\Lambda\Gamma^T$, $\mathrm{cov}[X_1, \ldots, X_n] = \Gamma(n)\Lambda(n)\Gamma(n)^T$.
- With eigenvectors
  $\Gamma = (\gamma_1, \ldots, \gamma_m)$, $\Gamma(n) = (\gamma_1(n), \ldots, \gamma_m(n))$ to
- eigenvalues
  $\lambda_1 \geq \ldots \geq \lambda_m \geq 0$, $\lambda_1(n) \geq \ldots \geq \lambda_m(n) \geq 0$, resp.,

Theorem (Asymptotic PCA, Anderson (1963); Watson (1983))

$E[\|X\|^4] < \infty$, λ_k *simple*, $\langle \lambda_k, \lambda_k(n) \rangle \geq 0$

$$\Rightarrow \sqrt{n}(\gamma_k(n) - \gamma_k) \xrightarrow{\mathbb{P}} \mathcal{N}\left(0, \sum_{k \neq j=1}^{m} \frac{\gamma_j \gamma_j^T \, \mathrm{cov}[XX']\gamma_k}{\lambda_k - \lambda_j}\right)$$

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Note, $\gamma_k \in \mathbb{S}^{m-1}$. Actually in $\mathbb{RP}^{m-1}$.
And, limiting distribution in $T_{\gamma_k} \mathbb{S}^{m-1} \cong T_{\pm\gamma_k} \mathbb{RP}^{m-1}$.

Non-Euclidean Descriptors

- Fréchet means
  - intrinsic (Kobayashi and Nomizu (1969); Bhattacharya and Patrangenaru (2003))
  - extrinsic (Hendriks and Landsman (1996); Bhattacharya and Patrangenaru (2003))
  - residual (Jupp (1988))
  - Procrustes (Gower (1975))
  - Ziezold (Ziezold (1994))
  - ⋮
- principal geodesics (Fletcher and Joshi (2004); H. et al 2010)
- principal submanifolds
  - (almost) totally geodesic (Jung et al. (2012): PN(G)S)
  - horizontal subspaces (Sommer (2016))
  - geodesic flows (Panaretos et al. (2014))
  - barycentric subspaces (Pennec (2017); Nye et al. (2016))
- flags of principal submanifolds (Pennec (2017))
- . . .

The CLT for Intrinsic Means on Manifolds

- M: m-dimensional Riemannian C^2 manifold
- d: intrinsic geodesic distance
- $X_1, \ldots, X_n \overset{\text{i.i.d.}}{\sim} X \in M$: random variables
- Fréchet (population) mean set:
  $E[X] = \operatorname{argmin}_{\mu \in M} \mathbb{E}[d(\mu, X)^2]$
- Fréchet (sample) mean set:
  $E_n[X_1, \ldots, X_n] = \operatorname{argmin}_{\mu \in M} \sum_{j=1}^{n} d(\mu, X_j)^2$
- $E[X] = \{\mu\}, \mu_n \in E_n[X_1, \ldots, X_n]$ measurable
- $\phi : M \to \mathbb{R}^m$ local C^2 chart near μ

Theorem (Bhattacharya and Patrangenaru (2005))

Under some additional regularity conditions

$$\sqrt{n}\big(\phi(\mu_n) - \phi(\mu)\big) \xrightarrow{\mathbb{P}} \mathcal{N}(0, \Sigma)$$

with suitable $\Sigma \geq 0$.

Idea of Proof

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Make a Mental Note

For the BP-CLT to hold, we need

(i) a C^2 manifold structure with C^2 distance^2 near

(ii) a unique population mean μ,

(iii) for all random $\hat{x}_n \overset{\text{a.s.}}{\to} 0$,

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Now a CLT for geodesics or more general subspaces?

Abstract Setup

- Random elements $X_1, \ldots, X_n \sim X$ ($n \in \mathbb{N}$) on a topological data space Q
- linked via a continous "distance" $\rho : Q \times P \to [0, \infty)$ to a topological descriptor space P, with continous $d : P \times P \to [0, \infty)$ vanishing exactly on diagonal,
- giving in P generalized Fréchet means

$$\text{population:} \quad E = \operatorname{argmin}_{p \in P} \mathbb{E}\big(\rho(X, p)^2\big)$$
$$\text{sample:} \quad E_n = \operatorname{argmin}_{p \in P} \sum_{j=1}^{n} \rho\big(X_j, p\big)^2 \quad .$$

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- (ρ, d) is a uniform link if

$$\forall p \in P, \epsilon > 0 \exists \delta = \delta(\epsilon, p) > 0 \text{ such that}$$
$$|\rho(x, p') - \rho(x, p)| < \epsilon \forall x \in Q, p' \in P \text{ with } d(p, p') < \delta.$$

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- (ρ, d) is a coercive link if $\exists p_0 \in P, C > 0$ such that $\forall p', p'_n, p_n \in P$ with $d(p_0, p_n) \to \infty \leftarrow d(p', p'_n)$

$$\rho(x, p_n) \to \infty \forall x \in Q \text{ with } \rho(x, p_0) < C;$$
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- Is the case if Q and P are compact.

The Two Strong Laws

Theorem (H. 2011b)

Ziezold Strong Consistency (cf. Ziezold (1977)) holds i.e.

$$\bigcap_{n=1}^{\infty} \overline{\bigcup_{k=n}^{\infty} E_k} \subset E \text{ a.s. },$$

if $\mathbb{E}\left(\rho(X,p)^2\right) < \infty \forall p \in P$, *Q separable,* (ρ, d) *uniform.*

Bhattacharya-Patrangenaru strong consistency (cf. Bhattacharya and Patrangenaru (2003)) holds if additionally $E \neq \emptyset$, (ρ, d) *coercive and* (P, d) *is Heine-Borel, i.e.* $\forall \epsilon > 0, \omega \in \Omega$ *a.s.* $\exists n = n(\epsilon, \omega) \in \mathbb{N}$ *such that*

$$\bigcup_{k=n}^{\infty} E_k \subset \{p \in P : d(E,p) \leq \epsilon\}.$$

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Theorem (H. 2011a)

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For $j \in \{1, \ldots, m\}$ and $k \in \{1, \ldots, j\}$,

$$f = \{p^j, \ldots, p^{j-k}\}, \text{ with } p^{l-1} \in S_{p^l}, l = j - k + 1, \ldots, j$$

is BNFD from P_j to P_{j-k} from the space

$$T_{j,k} = \left\{ f = \{p^{j-l}\}_{l=0}^{k} : p^{l-1} \in S_{p^l}, l = j - k + 1, \ldots, j \right\} ,$$

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For $j \in \{1, \ldots, m\}$ and $k \in \{1, \ldots, j\}$,

$$f = \{p^j, \ldots, p^{j-k}\}, \text{ with } p^{l-1} \in S_{p^l}, l = j - k + 1, \ldots, j$$

is BNFD from P_j to P_{j-k} from the space

$$T_{j,k} = \left\{ f = \{p^{j-l}\}_{l=0}^{k} : p^{l-1} \in S_{p^l}, l = j - k + 1, \ldots, j \right\} ,$$

with projection along each descriptor

$$\pi_f = \pi_{p^{m-k+1}, p^{m-k}} \circ \ldots \circ \pi_{p^m, p^{m-1}} : p^m \to p^{m-k}$$

Backward Nested Families of Descriptors

For another BNFD $f' = \{p'^{j-l}\}_{l=0}^{k} \in T_{j,k}$ set

$$d^j(f, f') = \sqrt{\sum_{l=0}^{k} d_j(p^{j-l}, p'^{j-l})^2}\,.$$

Backward Nested Fréchet Means

Random elements $X_1, \ldots, X_n \overset{\text{i.i.d.}}{\sim} X$ on a data space Q admitting BNFDs give rise to backward nested population and sample means (BN means) recursively defined via $f^m = \{Q\} = f_n^m$, i.e. $p^m = Q = p_n^m$ and for $j = m, \ldots, 1$,

$$p^{j-1} \in \operatorname*{argmin}_{s \in S_{p^j}} \mathbb{E}[\rho_{p^j}(\pi_{f^j} \circ X, s)^2], \qquad f^{j-1} = (p^k)_{k=j-1}^m$$

$$p_n^{j-1} \in \operatorname*{argmin}_{s \in S_{p_n^j}} \sum_{i=1}^n \rho_{p_n^j}(\pi_{f_n^j} \circ X_i, s)^2, \qquad f_n^{j-1} = (p_n^k)_{k=j-1}^m .$$

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If all of the population minimizers are unique, we speak of unique BN means.

Strong Law

Theorem (H. and Eltzner (2017))

If the BN population means $f = (p^m, \ldots, p^{m-k})$ *are unique and* $f_n = (p_n^m, \ldots, p_n^{m-k})$ *is a measurable selection of BN sample means then under "reasonable" assumptions*

$$f_n \to f \text{ a.s.}$$

i.e. $\exists \Omega' \subseteq \Omega$ *m'ble with* $\mathbb{P}(\Omega') = 1$ *such that* $\forall \epsilon > 0$ *and* $\omega \in \Omega'$, $\exists N(\epsilon, \omega) \in \mathbb{N}$

$$d(f_n, f) < \epsilon \quad \forall n \geq N(\epsilon, \omega)\,.$$

The Joint CLT [H. and Eltzner (2017)]

With local chart $\eta \overset{\psi^{-1}}{\mapsto} f^{j-1} \mapsto \rho_{p^j}(\pi_{f^j} \circ X, p^{j-1})^2 := \tau^j(\eta, X)$:

$$\sqrt{n} H_\psi \left(\psi(f_n^{j-1}) - \psi(f'^{j-1}) \right) \quad \to \quad \mathcal{N}(0, B_\psi) \, .$$

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Idea of proof:

$$0 \quad = \quad \operatorname{grad}_\eta \sum_{k=1}^{n} \tau^j(\eta_n, X_k) + \sum_{l=j+1}^{m} \lambda_n^l \operatorname{grad}_\eta \sum_{k=1}^{n} \tau^l(\eta_n, X_k)$$

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&\quad + \left(\operatorname{Hess}_\eta \sum_{k=1}^{n} \tau^j(\widetilde{\eta}_n, X_k) + \sum_{l=j+1}^{m} \lambda_n^l \operatorname{Hess}_\eta \sum_{k=1}^{n} \tau^l(\widetilde{\eta}_n, X_k) \right) \\
&\qquad \cdot (\eta' - \eta_n)
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with $\widetilde{\eta}_n$ between η' and η_n.

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&\qquad \cdot (\eta' - \eta_n)
\end{aligned}$$

with $\widetilde{\eta}_n$ between η' and η_n. N.B.: $\lambda_n^l \overset{\mathbb{P}}{\to} \lambda^l$.

The Joint Central Limit Theorem

With local chart $\eta \overset{\psi^{-1}}{\mapsto} f^{j-1} \mapsto \rho_{p^j}(\pi_{f^j} \circ X, p^{j-1})^2 := \tau^j(\eta, X)$:

$$\sqrt{n} H_\psi \left(\psi(f_n^{j-1}) - \psi(f'^{j-1}) \right) \quad \to \quad \mathcal{N}(0, B_\psi)$$

and typical regularity conditions, where

$$H_\psi \quad = \quad \mathbb{E}\left[\mathrm{Hess}_\eta \tau^j(\eta', X) + \sum_{l=j+1}^{m} \lambda^l \, \mathrm{Hess}_\eta \tau^l(\eta', X) \right] \text{ and}$$

$$B_\psi \quad = \quad \mathrm{cov}\left[\mathrm{grad}_\eta \tau^j(\eta', X) + \sum_{l=j+1}^{m} \lambda^l \, \mathrm{grad}_\eta \tau^l(\eta', X) \right] .$$

and $\lambda_{j+1}, \ldots \lambda_m \in \mathbb{R}$ are suitable such that

$$\mathrm{grad}_\eta \, \mathbb{E}\left[\tau^j(\eta, X)\right] + \sum_{l=j+1}^{m} \lambda^l \, \mathrm{grad}_\eta \, \mathbb{E}\left[\tau^l(\eta, X)\right]$$

vanishes at $\eta = \eta'$.

Factoring Charts

If the following diagram commutes we say the chart factors

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\begin{array}{ccccccccc}
T_{m-1,j-1} & \ni & f^{j-1} & = & (f^j, p^{j-1}) & \xrightarrow{\psi} & \eta & = & (\theta, \xi) \\
 & & & & \downarrow \pi^{P_{j-1}} & & & & \downarrow \pi^{\mathbb{R}^{\dim(\theta)}} \\
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Taylor expansion at $\eta' = (\theta', \xi')$ gives a joint Gaussian CLT,

$$\sqrt{n} H_\psi(\eta_n - \eta') = \sqrt{n} H_\psi \begin{pmatrix} \theta_n - \theta' \\ \xi_n - \xi' \end{pmatrix} \quad \to \quad \mathcal{N}(0, B_\psi)$$

and projection to the θ coordinate preserves Gaussianity.

BNFD CLT Incl. Factoring Charts

Holds for (Eltzner and H. 2017)

- PNS,PNGS.
- 1st geodesic PC on manifolds including intrinsic mean on 1st PC,
- 1st geodesic PC on Kendall shape spaces (notably not a manifold beginning with dim 3) including intrinsic mean on 1st PC,
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Practioner's advice:

- For a two-sample test, need empirical covariances.
- Suitably bootstrap data (Eltzner and H. 2017).

Revisiting "Typical Regularity Conditions" I

Recall conditions

(i) a C^2 manifold structure with C^2 distance^2 near

(ii) a unique population mean μ,

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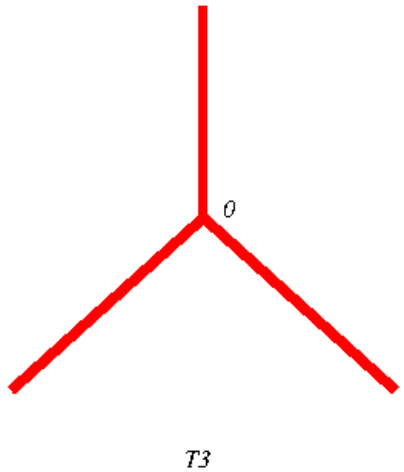

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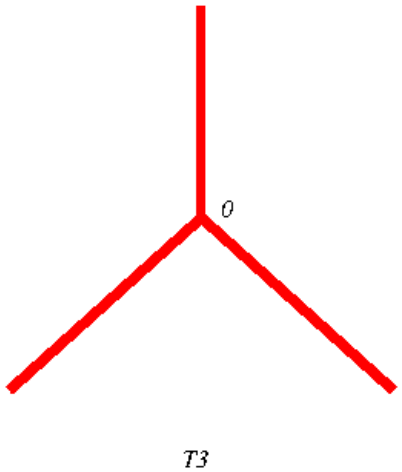

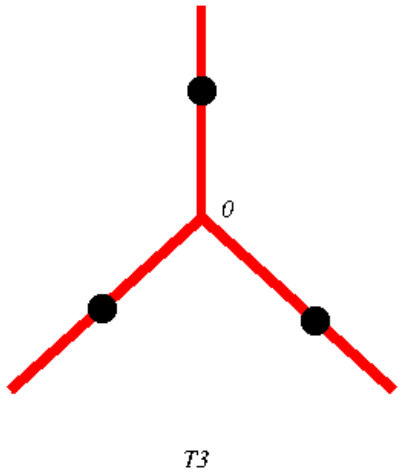

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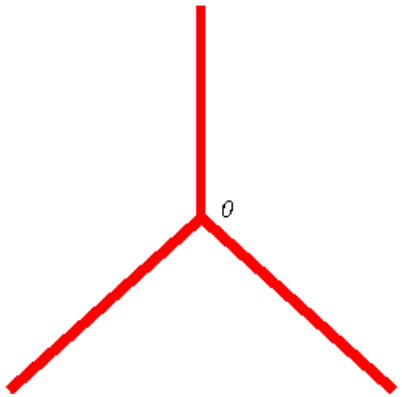

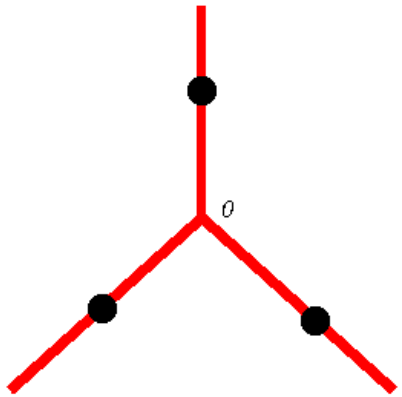

T3

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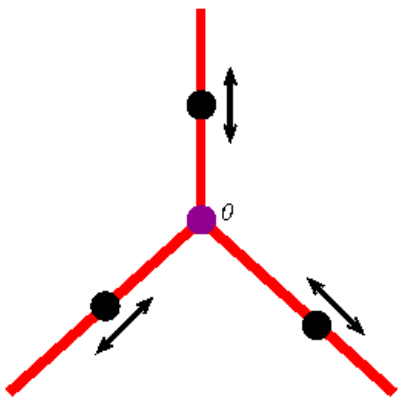

d(three points)

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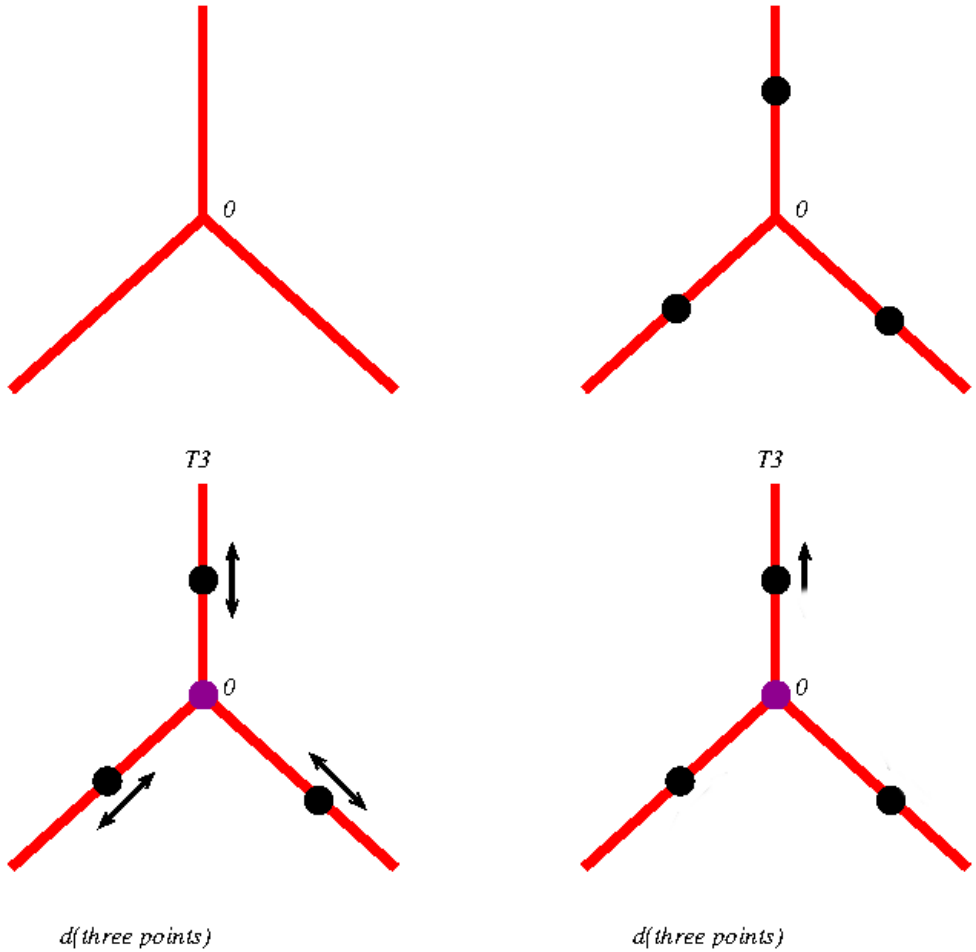


Hotz et al. (2013)

A General Definition for Stickiness

Let $\mathcal{M}$ be a set of measures on a metric space (Q, ρ). Assume $\mathcal{M}$ has a given topology. A mean is a continuous map

$$\mathcal{M} \to \{\text{closed subsets of } Q\}.$$

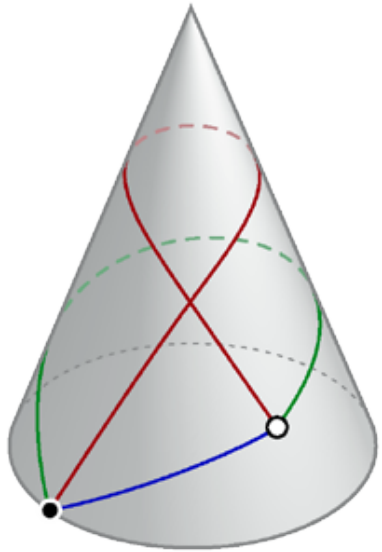
A measure μ sticks to a closed subset $C \subset Q$ if every neighborhood of μ in $\mathcal{M}$ contains a nonempty open subset consisting of measures whose mean sets are contained in C.

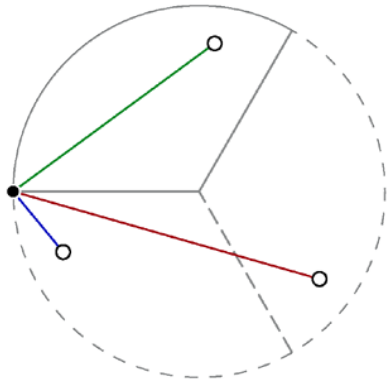
Typical topology by Wasserstein metric

$$\rho(\mu, \nu) = \sup_{f \in \mathrm{Lip}_1(\mathcal{K}, \mathbb{R})} \left(\int f \, d\mu - \int f \, d\nu \right),$$

(H. et al. 2015).

Example: The Cone





Exercise

Unless $X =$ cone point a.s., $E^{\rho} \neq$ cone point.

The Hyperbolic Cone

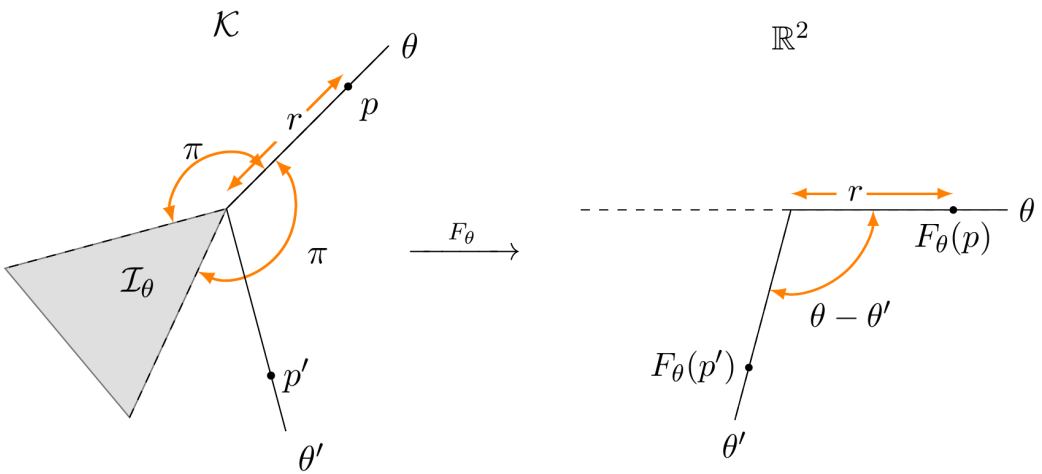
- opening angle $\alpha > 2\pi$
- contains way more ice cream

The Hyperbolic Cone

- opening angle $\alpha > 2\pi$
- contains way more ice cream
- can be embedded in $\mathbb{R}^3$ only non-isometrically, say, as a kale

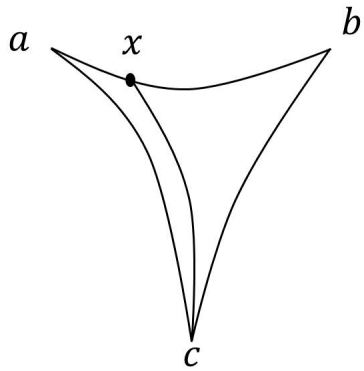
$$\mathcal{K} = ([0, \infty) \times [0, \alpha])/\sim$$

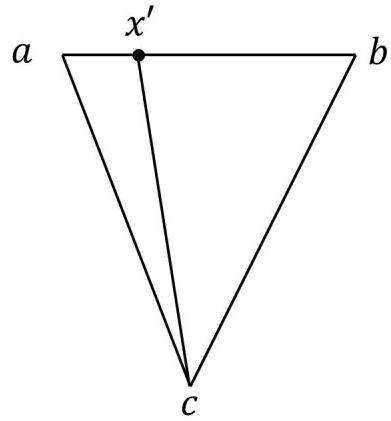
- polar coordinates $p = (r, \theta) \in [0, \infty) \times [0, \alpha]/\sim$
- folding map F_θ



Uniqueness of Fréchet Means Under Non-Positive Curvature

A metric space (Q, ρ) is NPC if every ρ-triangle mapped to $\mathbb{R}^2$ is more skinny, i.e., ρ-distances accross are smaller than corresponding Euclidean distances





Theorem (Sturm (2003))

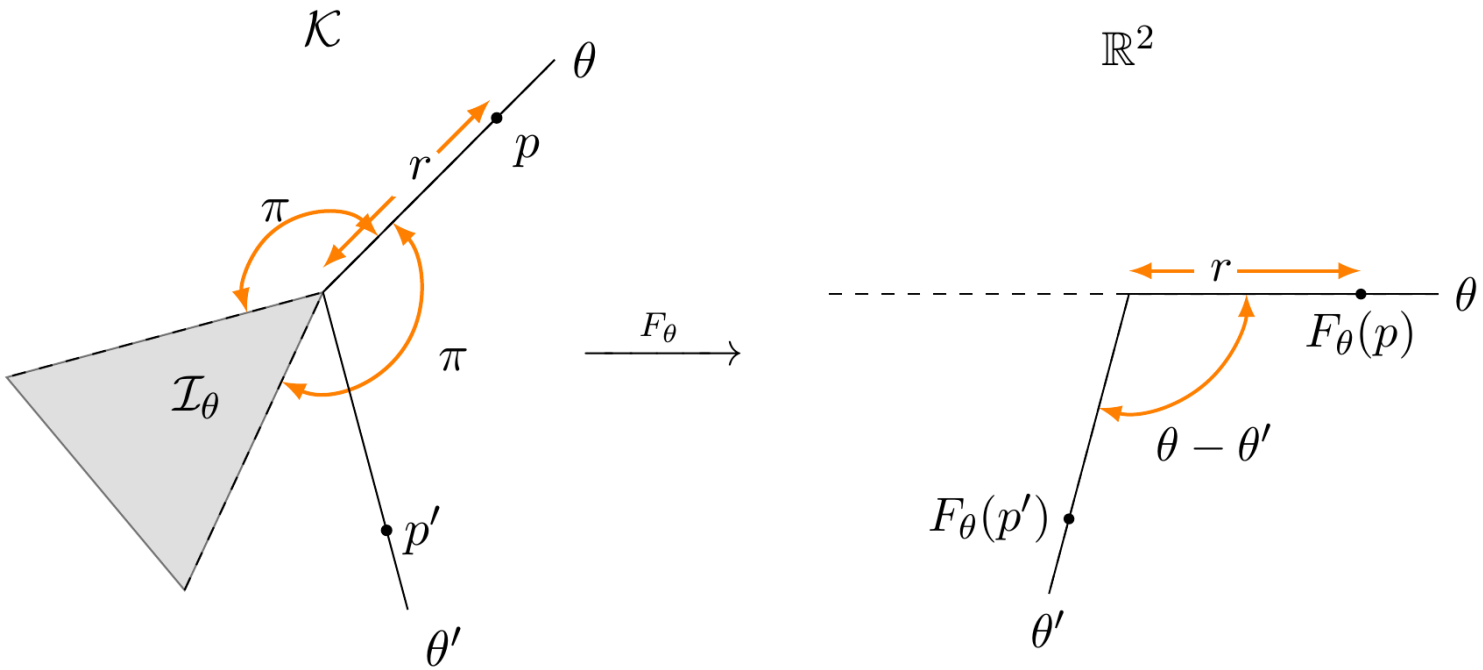
On a complete NPC metric space, Fréchet means are unique.

Notation: $\{\mu_n\} := E_n^\rho$, $\{\mu\} := E^\rho$.

Folded Moments

Recall the folding map

$$F_\theta(r', \theta') = \begin{cases} \mathbf{0} & \text{if } r' = 0 \\ \left(r' \cos(\theta' - \theta), r' \sin(\theta' - \theta)\right) & \text{if } \left|\theta' - \theta\right| < \pi \text{ and } r' > 0 \\ (-r', 0) & \text{if } \left|\theta' - \theta\right| \geq \pi \text{ and } r' > 0. \end{cases}$$



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in conjunction with a measure $\mathbb{P}^X$ on $\mathcal{K}$, giving rise to folded moments

$$m_\theta = \int_{\mathcal{K}} F_\theta(p) \, d\,\mathbb{P}^X(p)$$

Key feature: Under integrability $\int_{\mathcal{K}} \rho(\mathbf{0}, p) \, d\,\mathbb{P}^X(p) < \infty$,

$$\frac{d}{d\theta} m_{\theta,1} = m_{\theta,2}$$

(derivative is zero on the shadow and so is $m_{\theta,2}$).

The Shadow's (Boundary) Effect

$$D_\theta^{\pm}\frac{dm_{\theta,1}}{d\theta} = D_\theta^{\pm} m_{\theta,2} = -m_{\theta,1} + \int_{\mathcal{I}_\theta^{\mp}} \big(-\rho(\mathbf{0},p)\big)\, d\,\mathbb{P}^X(p)$$

$$\leq -m_{\theta,1} - \int_{\mathcal{I}_\theta} \rho(\mathbf{0},p)\, d\,\mathbb{P}^X(p)$$

with

$$\mathcal{I}_\theta^+ = \mathcal{K} \setminus \{(r,\theta') \mid r > 0 \text{ and } -\pi \leq \theta' - \theta < \pi\},$$
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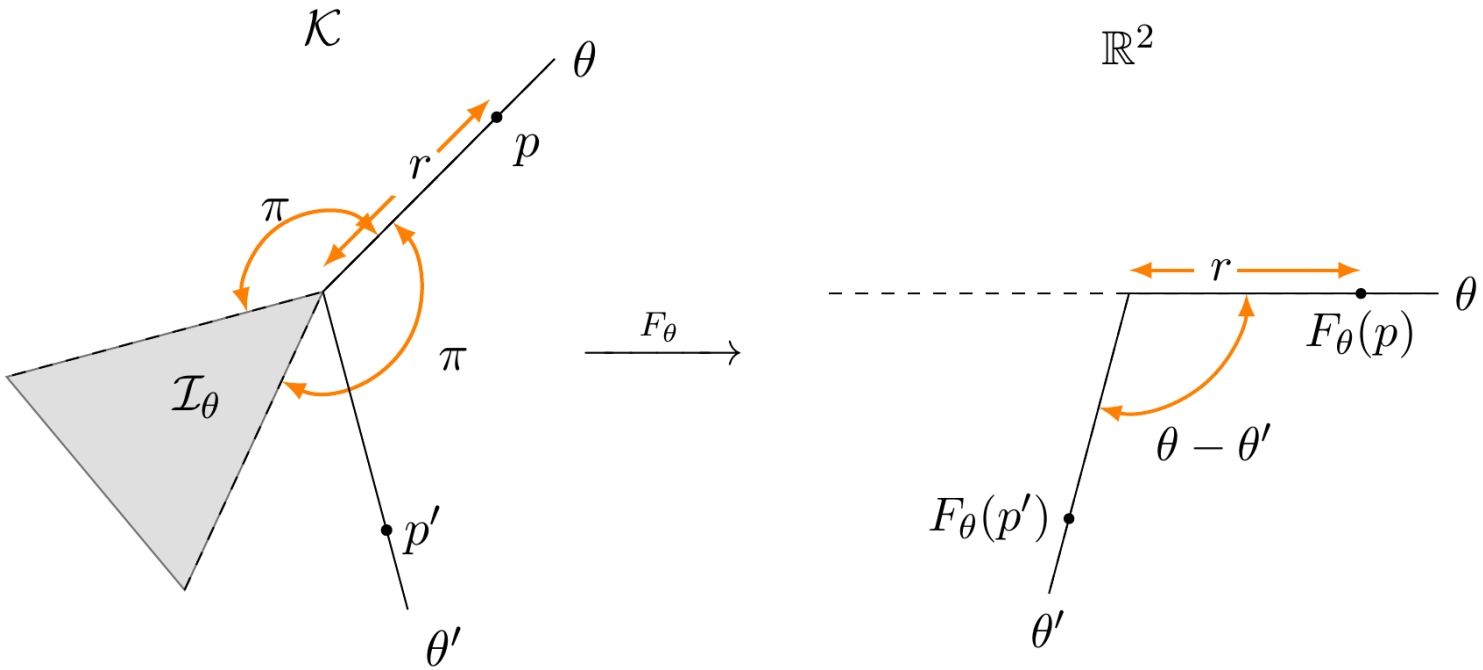

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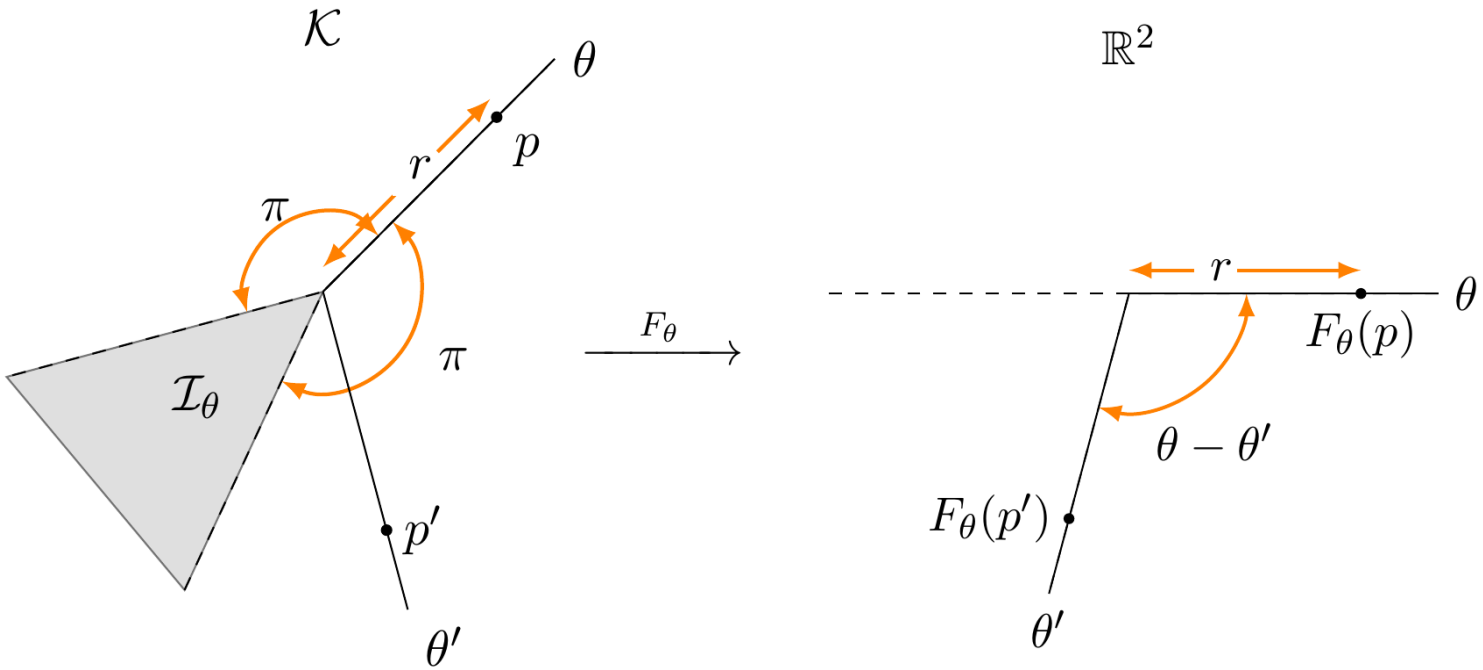

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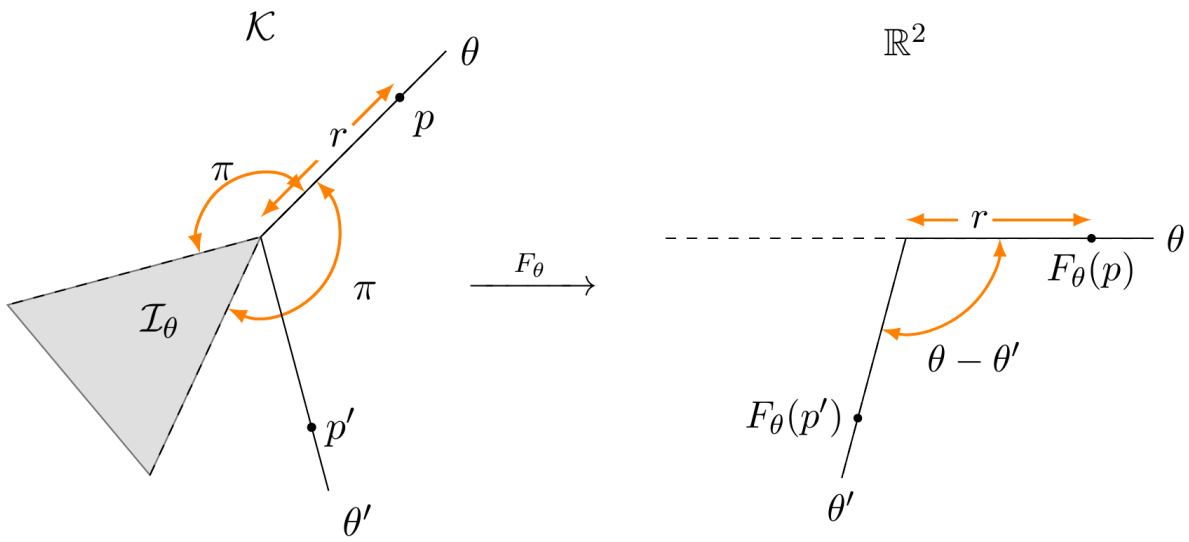

$$m_{\theta,1} \leq -m_{\theta',1} \quad \forall (1,\theta') \in \mathcal{I}_\theta\,.$$

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$$\Downarrow$$

Lemma

Let $A \neq B$ and $m_{\theta,1} \geq 0$ on $\theta \in [A,B]$. Then $|A-B| \leq \pi$.

- *if $m_{\theta,1} = 0\ \forall \theta \in [A,B] \Rightarrow \mathbb{P}^X(\mathcal{I}_\theta) = 0\ \forall \theta \in [A,B]$.*
- *if $m_{\theta,1} > 0$ then it's concave there.*

The Strong Law

Theorem

Assuming integrability and nondegeneracy,

$$1_{\{m_{\theta,1} \geq 0\}} \subset [0, \alpha]/\sim \text{ is a closed interval, or empty}$$

that is exactly one of the following:

(fully sticky) *empty, then* $\mu = \mathbf{0}$ *and* $\exists n^*(\omega) \in \mathbb{N}$ *such that* $\mu_n(\omega) = \mathbf{0}$ *for all* $n \geq n^*(\omega)$, *a.s.*

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(partly sticky) *of length* $< \pi$*, with* $m_{\theta,1} = 0$ *on its entirety such that* $\mu = \mathbf{0}$ *and* $\mu_n(\omega) \to \mathbf{0}$ *a.s.*
Furthermore, if $1_{\{m_{\theta,1} \geq 0\}} \subset (A, B)$
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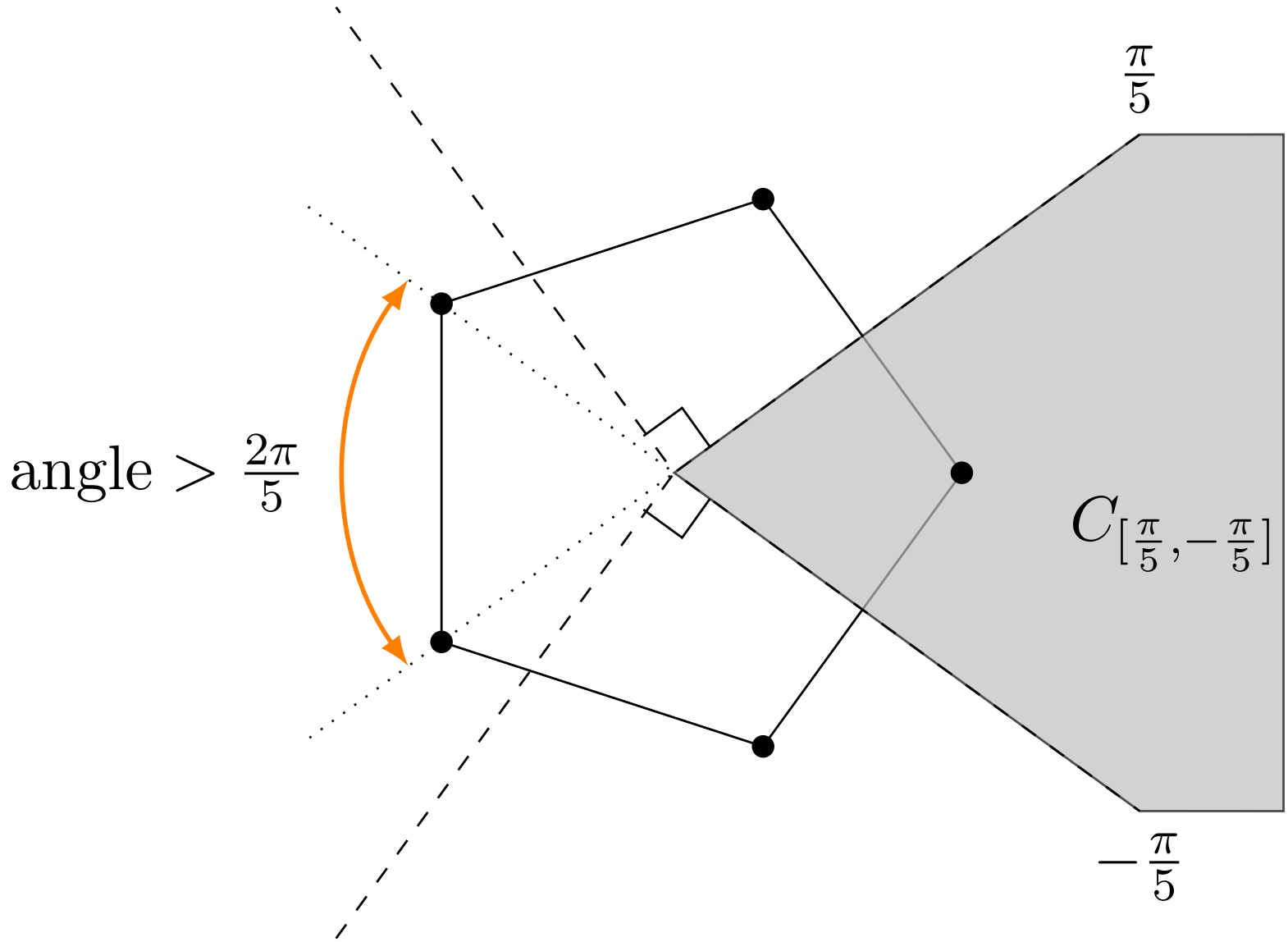
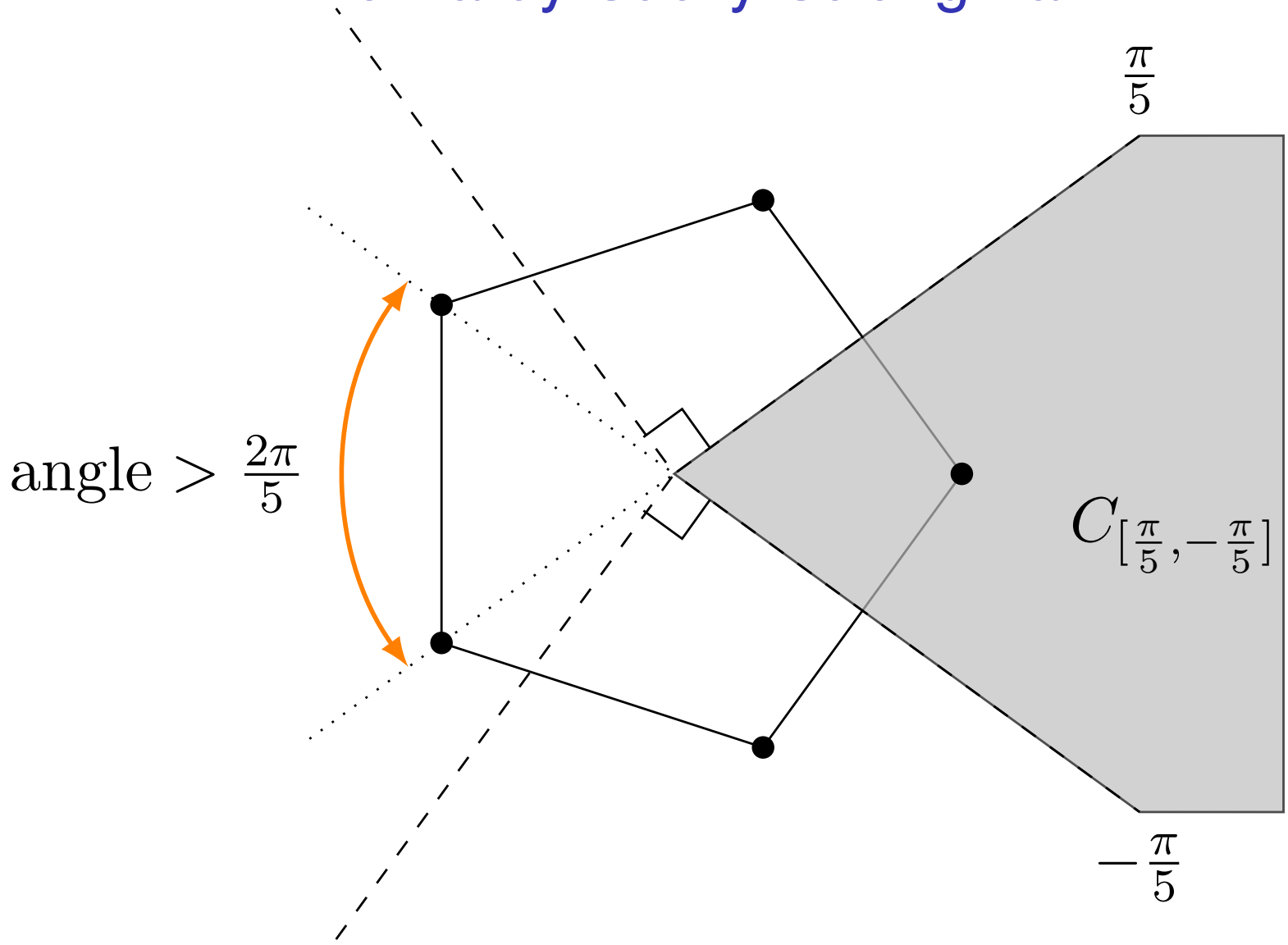
(nonsticky) *of length* $\leq \pi$*, with* $m_{\theta,1}$ *strictly concave (and hence strictly positive) on its interior.*
$\mu_n(\omega) \to \mu \neq \mathbf{0}$ *a.s.*

The Partly Sticky Strong Law



Uniformly sampling from a pentagon's vertices

The Partly Sticky Strong Law



For the uniform on $\{(r,\theta) : -\pi < \theta < \pi\}$ the fluctuation is only on $[0,\infty)$

Sticky CLTs on the Kale

1. Fully sticky $\Rightarrow$ trivial CLT ✓
2. Partly sticky $\Rightarrow$??
3. Nonsticky $\Rightarrow$ BP-CLT (classical $\sqrt{n}$ Gaussian)?

The Partly Sticky CLT

In case of square integrability and $1_{\{m_{\theta,1}\geq 0\}} = [A, B] = 1_{\{m_{\theta,1}=0\}}$ *(recall length* $< \pi$*), with center* θ^**, decompose suitable Gaussian in* $\mathbb{R}^2$ *centered at* $\mathbf{0}$ *into three parts:*

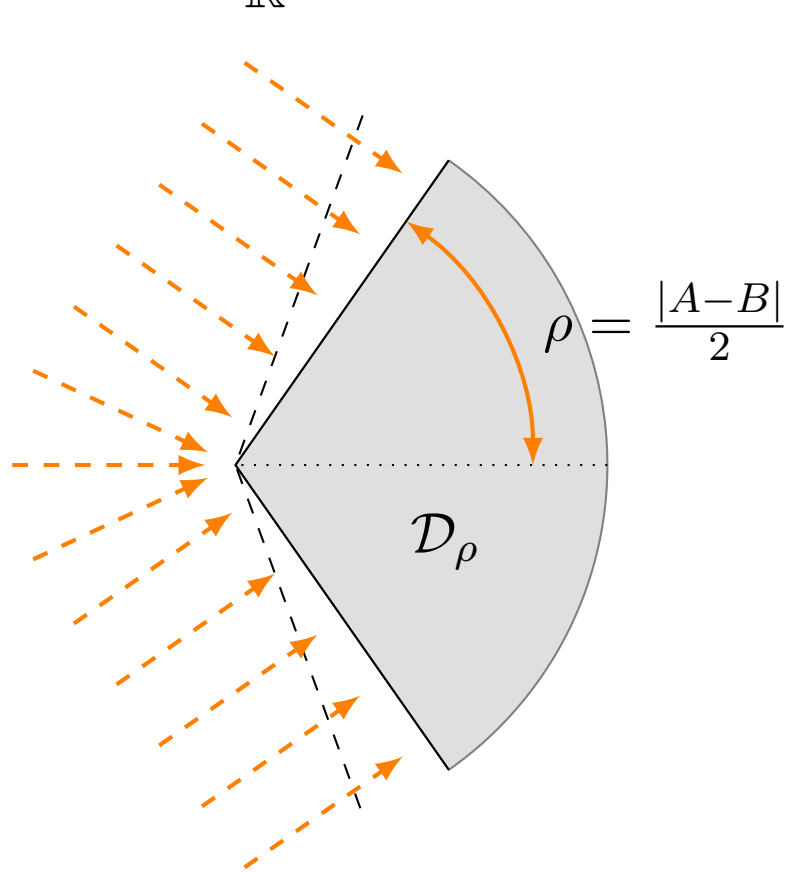
- $\mathcal{G}_1$ *in cone* D_ρ*,*
- $\mathcal{G}_2$ *in the two adjacent cones with* 90^0 *opening,*
- $\mathcal{G}_3$ *in the rest.*

The limiting distribution of

$$\sqrt{n}\big(F_{\theta^*}(\mu_n) - \mathbf{0}\big)$$

is

$$\mathcal{G}_1 + \pi_{C_A \cup C_B} \circ \mathcal{G}_2 + \pi_{\mathbf{0}} \circ \mathcal{G}_3 \,.$$



The Nonsticky CLT

In case of square integrability and $\mu = (r^*, \theta^*)$, $r^* > 0$, *define*

$$\kappa(\omega) = \begin{cases} \dfrac{\int_{\mathcal{I}^+_{\theta^*}} \rho(\mathbf{0}, p)\, d\,\mathbb{P}^X(p)}{r^*} & \text{if } e_2 \cdot F_{\theta^*}\mu_n(\omega) < 0 \\ \dfrac{\int_{\mathcal{I}^-_{\theta^*}} \rho(\mathbf{0}, p)\, d\,\mathbb{P}^X(p)}{r^*} & \text{if } e_2 \cdot F_{\theta^*}\mu_n(\omega) > 0, \end{cases}$$

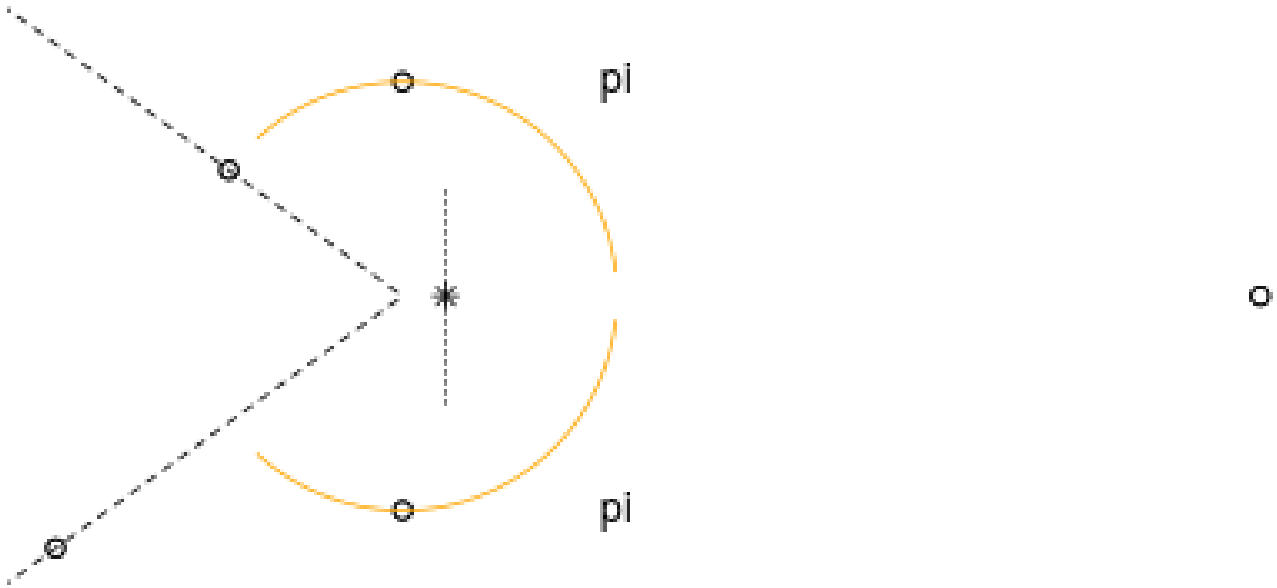
and

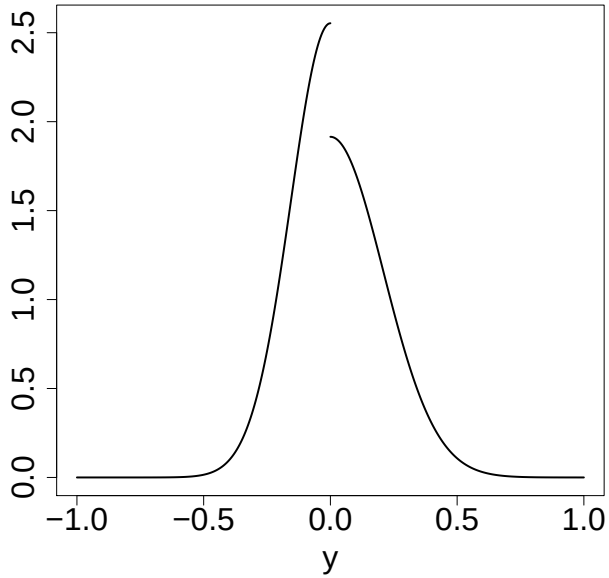
$$Q_n(W) = \mathbb{P}\left\{\left(\sqrt{n}(e_1 \cdot F_{\theta^*}\mu_n - r^*, (1+\kappa)e_2 \cdot F_{\theta^*}\mu_n\right) \in W\right\}.$$

Then, $Q_n \to \mathcal{G}$ *weakly where* $\mathcal{G}$ *is a suitable Gaussian in* $\mathbb{R}^2$ *centered at* $(r^*, 0)$ *with covariance*

$$\int_{\mathbb{R}^2} (y - F_{\theta^*}\mu)(y - F_{\theta^*}\mu)^T\, d\,\mathbb{P}^X \circ F^{-1}_{\theta^*}(y)\,.$$

Example of Non-Gaussian Nonsticky CLT





Curiosities and Motivation

- The fully sticky CLT only requires integrability.
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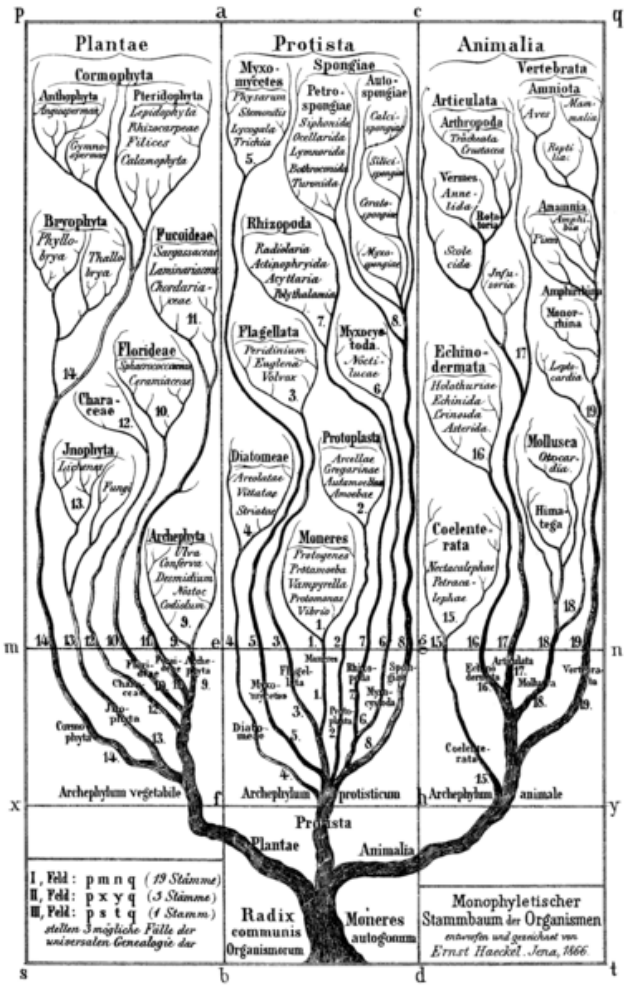
- This research has been motivated by statistical analysis of phylogenetic trees, the famous BHV tree space (Billera et al. (2001)) has a hyperbolic singularity at the cone point = star tree.



Tree of Evolution by Haeckel (1879)

Revisiting "Typical Regularity Conditions" II

Recall conditions

(iii) for all random $\hat{x}_n \overset{\text{a.s.}}{\to} 0$, $\text{Hess}|_{x=\hat{x}_n} F_n(x) \overset{\mathbb{P}}{\to} \text{Hess}|_{x=0} F(x)$,

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Theorem (Eltzner and H. 2018)

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Theorem (Eltzner and H. 2018)

$\sqrt{n}\,\phi(\hat{p}_n)^r \xrightarrow{\mathcal{D}} \mathcal{N}(0, \Sigma)$ (power component-wise), suitable $\Sigma > 0$. $\phi(\hat{p}_n)$ has rate $n^{-\frac{1}{2(r-1)}}$, is $r - 2$-smeary.

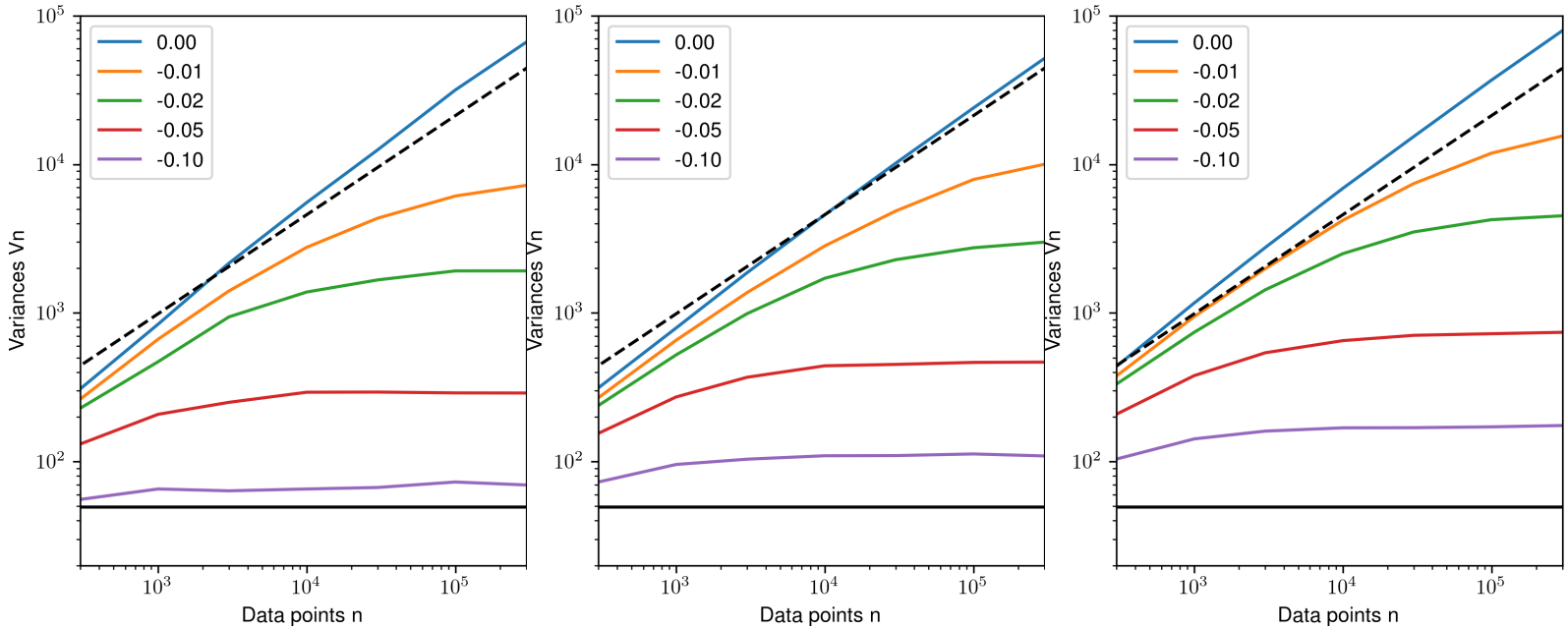
k-Smeariness

If

$$n^{\frac{1}{2(k+1)}}\left(\phi(\hat{p}_n) - \phi(p)\right)$$

has a non-trivial distribution as $n \to \infty$.

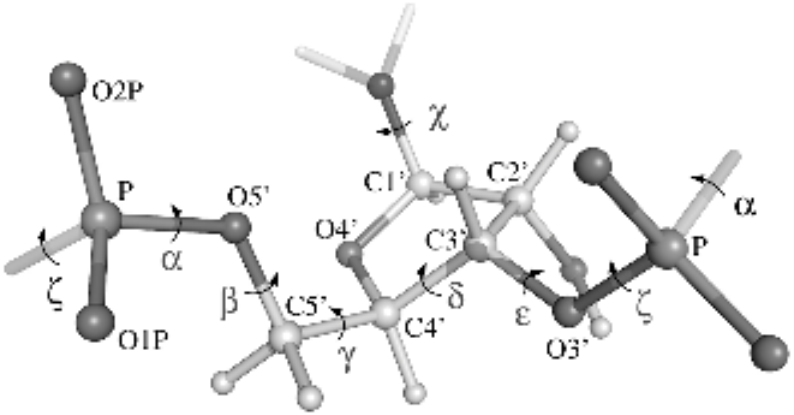
- $k = 2$ smeary (dashed line)

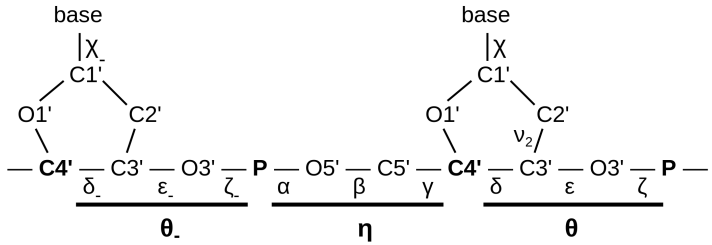


On a sphere $\mathbb{S}^m$ with dimension (all derivatives $O(m^{-1/2})$)

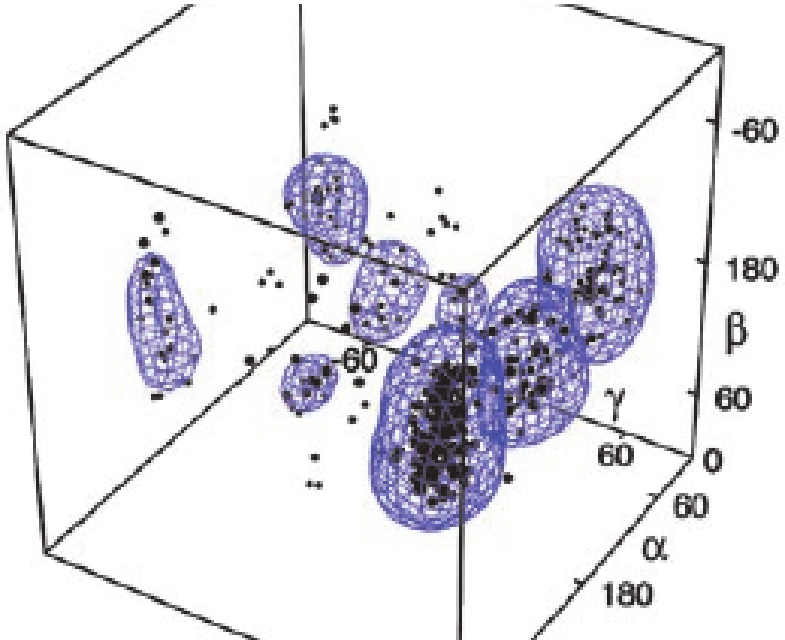
$m = 2$ $m = 10$ $m = 100$

Dimension Reduction in RNA Structure Analysis





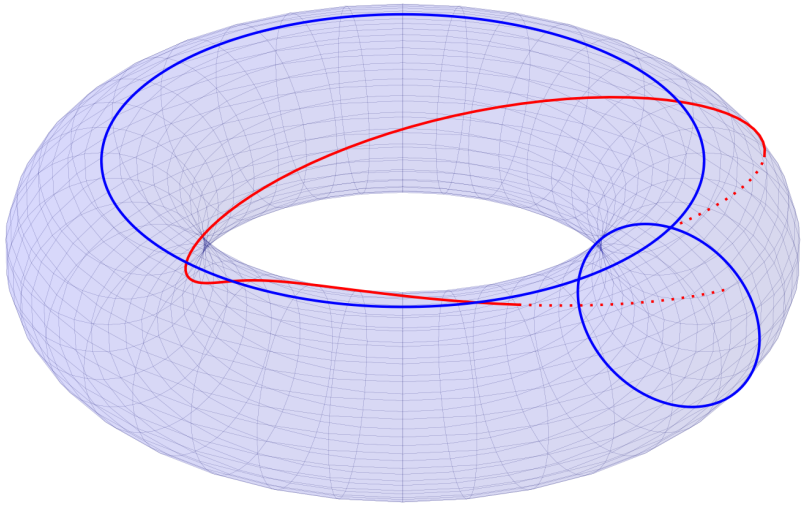
- 7 dihedral angles $\in (\mathbb{S}^1)^7$, 2 pseudotorsion angles $\in (\mathbb{S}^1)^2$,
- = shape, i.e. translational / rotational invariant

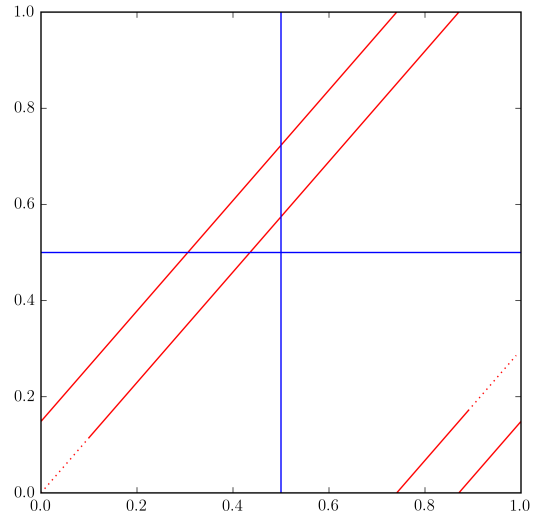


- Murray et al. (2003) using www.rscb.org:
- C2'-pucker RNA clusters in many 1D groups in heminucleotide angles.
- Can we verify (improve? understand?) by PCA?

PCA on a Torus $\mathbb{S}^1 \times \ldots \times \mathbb{S}^1$

- Only very few geodesics are not winding around,
- an uncountable number of geodesics is dense and
- every data set can be perfectly approximated.
- Standard geometry of $(\mathbb{S}^1)^k$ is not statistically benign.





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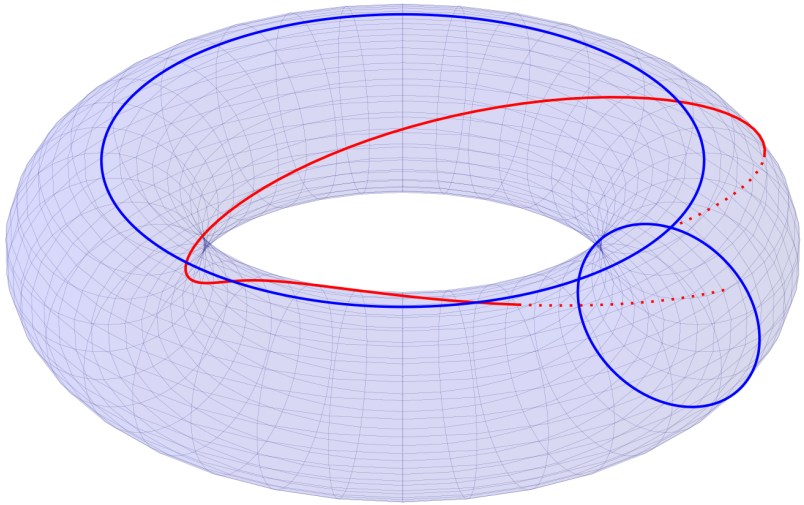

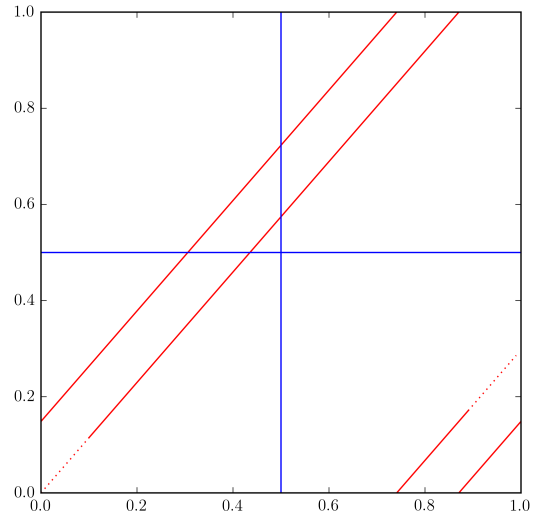

- Altis et al. (2008); Kent and Mardia (2009, 2015) allow only few geodesics.
- Tangent space PCA (Euclidean) for $(\mathbb{S}^1)^k$ "$\subset$" $\mathbb{R}^k$.
- Dihedral PCA Altis et al. (2008); Sargsyan et al. (2012) $(\mathbb{S}^1)^k \subset \mathbb{R}^{2k}$.

Euclidean vs. Spherical PCA

P_k = all "canonical" k-dim. subspaces in m-dim. Q.

$\dim(P_k)$

- $= \dim G(m,k) + \sharp$ translates
  $= (m-k)k + m - k = (m-k)(k+1)$ for $Q = \mathbb{R}^m$,
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- $= \dim G(m+1,k+1) + (m-k) = (m-k)(k+2)$ for $Q = \mathbb{S}^m$, small subspheres, non-nested, statistically more benign than Euclidean PCA.

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$\dim(P_k)$

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  $= (m-k)k + m - k = (m-k)(k+1)$ for $Q = \mathbb{R}^m$, canonically nested,
- $= \dim G(m+1,k+1) = (m-k)(k+1)$ for $Q = \mathbb{S}^m$, great subspheres, non-nested,
- $= \dim G(m+1,k+1) + (m-k) = (m-k)(k+2)$ for $Q = \mathbb{S}^m$, small subspheres, non-nested, statistically more benign than Euclidean PCA.

- make this nested $\rightarrow$ principal nested (great)subspheres (PN(G)S) by Jung et al. (2012).

Sausage Transformation

$(\mathbb{S}^1)^k \to \mathbb{S}^k$?

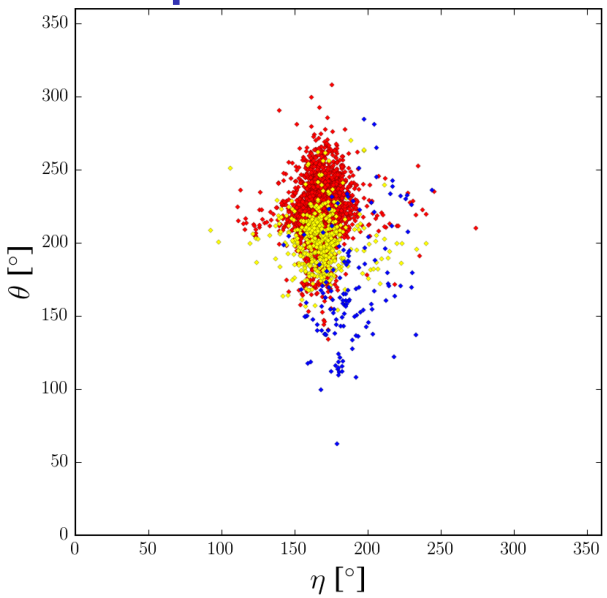
Data Driven Torus (T) PCA for $(\mathbb{S}^1)^k$

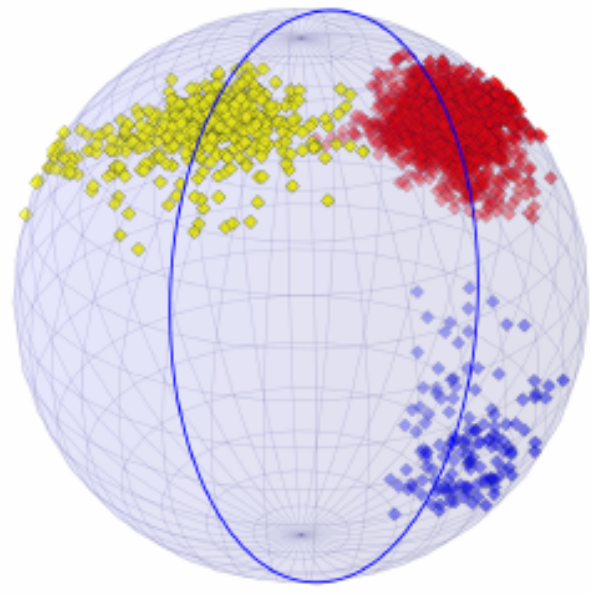
- Choose a codimension 2 subtorus furthest from data (opposite to mean, or largest gap) $\to \mathbb{S}^k/\sim$ glued along "that" $\mathbb{S}^{k-2}$,
- ideally, data near equatorial circle (EC) orthogonal (no deformation),
- center and number new angles by highest variance inside, or outside,

$$\sum_{l=1}^{k} d\psi_l^2 \to d\phi_1^2 + \sum_{l=2}^{k} \left(\prod_{j=1}^{l-1} \sin^2 \phi_j \right) d\phi_l^2 \,,$$

- halve all angles (but the last) – otherwise we obtain several copies of $\mathbb{S}^k/\sim$ glued together,
- do a variant of PNS (non-glued small subspheres, optimized by $\mathbb{S}^k/\sim$ distance).

Separation of Clusters by 7D Torus PCA

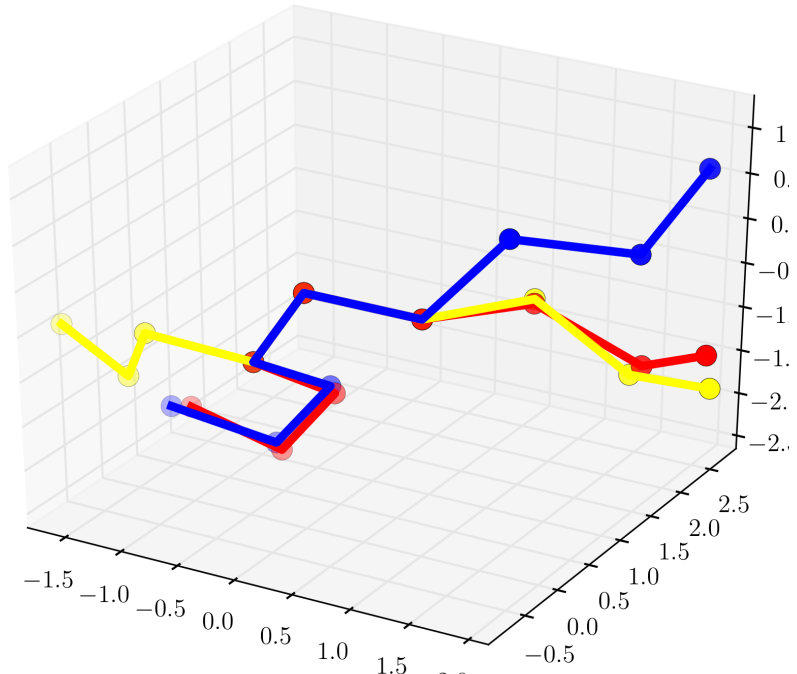




1: α-helix well known

2: helical-like less known

7: low-density new



Wrap UP: Challenges

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Thank you!

IMo1GPCs Give Factoring Charts

$$P_2 = \{Q\},\ S_Q = P_1 = \left\{ [\gamma_{q,v}] : \left(q, \pm \frac{v}{\|v\|} \right) \in PQ \right\} / \sim,\ P_0 = Q\,.$$

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$$\begin{aligned} T_{1,1} = \{(p,s) : p = [\gamma_{q,v}] \in P_1,\ s \in p\} &\to PQ, \\ ([\gamma_{q,v}], s) &\mapsto (s, \{w, -w\}) \end{aligned}$$

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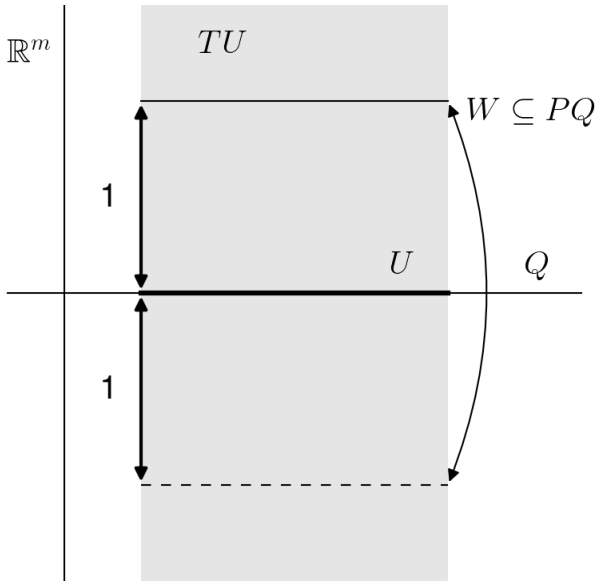

$PQ =$ projective bundle.
Local trivialization of the tangent bundle

$$TU = U \times \mathbb{R}^m$$

gives local trivialization of the projective bundle and thus factoring charts.

$$T_{1,1} = \{(p, s) : p = [\gamma_{q,v}] \in P_1,\ s \in p\} \rightarrow PQ,$$
$$([\gamma_{q,v}], s) \mapsto (s, \{w, -w\})$$

The PNS/PNGS Framework

$$\mathbb{S}^m \supset \underbrace{p^{m-1}}_{\in P_{m-1}} \supset \ldots \supset \underbrace{p^1}_{\in P_1} \supset \underbrace{p^0}_{\in P_0}, \quad f^j = (p^{m-1}, \ldots, p^j)$$

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$$O(j+1, m+1) = \left\{ \underbrace{(v_1, \ldots, v_{m-j})}_{=v} \in \mathbb{R}^{(m+1)\times(m-j)} : \right.$$

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S_p &= \left\{ \begin{bmatrix} v, v_{m-j+1} \\ \alpha^T, \alpha_{m-j+1} \end{bmatrix} : v_{m-j+1} \in \mathbb{S}^m, \alpha_{m-j+1} \in \mathbb{R} \text{ with} \right. \\
&\qquad \left. v_{m-j+1}^T v = 0, \alpha_{m-j+1}^2 < 1 - \|\alpha\|^2 \right\} \\
&\subseteq P_{j-1} \text{ for } p = [v^T, \alpha]^T \in P_j .
\end{aligned}$$

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\end{aligned}$$

For PNGS, $\alpha = 0 = \alpha_{m-j+1}$.

Chart Factoring for PNS/PNGS

$$S_p = \left\{ \begin{bmatrix} V, v_{m-j+1} \\ \alpha^T, \alpha_{m-j+1} \end{bmatrix} : v_{m-j+1} \in \mathbb{S}^m, \alpha_{m-j+1} \in \mathbb{R} \dots \right\}$$

Chart Factoring for PNS/PNGS

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Lemma

For every $z' = \begin{pmatrix} v', v'_{m-j+1} \\ \alpha'^T, \alpha'_{m-j+1} \end{pmatrix} \in M_{j-1}$, $\exists \epsilon > 0$ *such that*

$$U_{j-1}^{z'} := \left\{ z \in M_{j-1} : z^T z' - z'^T z = 0, \|z - z'\| < \epsilon \right\}$$

is locally diffeomorphic with P_{j-1} *near* $[z'] = s'$.

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Theorem

$$T_{j,1} = \{(p, s) : s \in S_p \subseteq P_{j-1}, p \in P_j\}$$

has a factoring chart near (p', s')

$$(p, s) \rightarrow (z, b) \in U_{j-1}^{z'} \times \mathbb{S}^{m-j}$$

with $s = [z], p = [Bz]$, $(b, B) \in O(m - j + 1)$.

Two-Sample Descriptor Test

$$
\begin{array}{lccccc}
\text{Data:} & \underbrace{X_1, \ldots, X_n} & , & \underbrace{Y_1, \ldots, Y_m} & \in & Q \\
 & \downarrow & & \downarrow & & \\
\text{Descriptors:} & f^X, p^X & & f^Y, p^Y & \in & T, P \\
 & \downarrow & \phi & \downarrow & & \\
\text{Coordinates:} & Z^X & & Z^Y & \in & \mathbb{R}^D
\end{array}
$$

Two-Sample Descriptor Test

$$\begin{array}{lccc} \text{Data:} & \underbrace{X_1, \ldots, X_n} \quad , \quad \underbrace{Y_1, \ldots, Y_m} & \in & Q \\ & \downarrow \qquad\qquad \downarrow & & \\ \text{Descriptors:} & f^X, p^X \qquad\quad f^Y, p^Y & \in & T, P \\ & \downarrow \qquad \phi \qquad \downarrow & & \\ \text{Coordinates:} & Z^X \qquad\quad Z^Y & \in & \mathbb{R}^D \end{array}$$

Under $H_0 : X \sim Y$,

$$\frac{nm}{n+m}(m+n-2)(Z^X - Z^Y)^T \left(n\,\widehat{\text{cov}}[Z^X_{1\ldots n}] + m\,\widehat{\text{cov}}[Z^Y_{1\ldots m}] \right)^{-1} \cdot (Z^X - Z^Y) \sim \mathcal{T}^2(k, n+m-2)$$

Two-Sample Descriptor Test

$$\begin{array}{lccc} \text{Data:} & \underbrace{X_1, \ldots, X_n} \quad , \quad \underbrace{Y_1, \ldots, Y_m} & \in & Q \\ & \downarrow \qquad\qquad \downarrow & & \\ \text{Descriptors:} & f^X, p^X \qquad\quad f^Y, p^Y & \in & T, P \\ & \downarrow \qquad \phi \qquad \downarrow & & \\ \text{Coordinates:} & Z^X \qquad\quad Z^Y & \in & \mathbb{R}^D \end{array}$$

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But how to access $\widehat{\text{cov}}[Z^X_{1\ldots n}]$ and $\widehat{\text{cov}}[Z^Y_{1\ldots m}]$?

Bootstrapping

For $b = 1, \ldots, B$, resample:

- $X^*_{1,b}, \ldots, X^*_{n,b}$ from $X_1, \ldots, X_n$ gives $\widehat{\mathrm{cov}}[Z^X_{1\ldots n}]$

Bootstrapping

For $b = 1, \ldots, B$, resample:

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- $Y^*_{1,b}, \ldots, Y^*_{m,b}$ from $Y_1, \ldots, Y_m$ gives $\widehat{\text{cov}}[Z^Y_{1\ldots m}]$
- set $A = n\widehat{\text{cov}}[Z^X_{1\ldots n}] + m\widehat{\text{cov}}[Z^Y_{1\ldots m}]$

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Again, for $b = 1, \ldots, B'$, resample:

- $W^*_{1,b}, \ldots, W^*_{n+m,b}$ from $X_1, \ldots, X_n, Y_1, \ldots, Y_m$

Bootstrapping

For $b = 1, \ldots, B$, resample:

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- set $X^*_{j,b} = W^*_{j,b}$ for $j = 1, \ldots, n$

Bootstrapping

For $b = 1, \ldots, B$, resample:

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- $Y^*_{1,b}, \ldots, Y^*_{m,b}$ from $Y_1, \ldots, Y_m$ gives $\widehat{\mathrm{cov}}[Z^Y_{1\ldots m}]$
- set $A = n\,\widehat{\mathrm{cov}}[Z^X_{1\ldots n}] + m\,\widehat{\mathrm{cov}}[Z^Y_{1\ldots m}]$

Again, for $b = 1, \ldots, B'$, resample:

- $W^*_{1,b}, \ldots, W^*_{n+m,b}$ from $X_1, \ldots, X_n, Y_1, \ldots, Y_m$
- set $X^*_{j,b} = W^*_{j,b}$ for $j = 1, \ldots, n$
- set $Y^*_{j,b} = W^*_{j+n,b}$ for $j = 1, \ldots, m$

Bootstrapping

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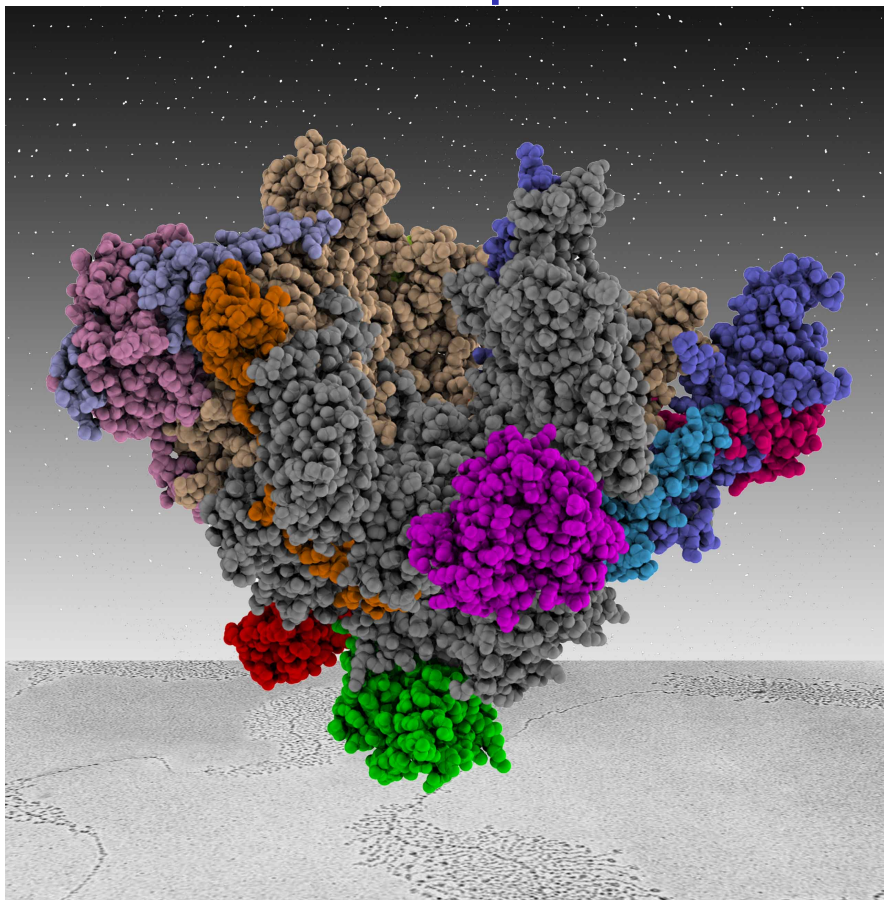
Then, the test

$$\textit{reject } H_0 \textit{ if } (Z^X - Z^Y)^T A^{-1} (Z^X - Z^Y) > c^*_{1-\alpha}$$

has the asymptotic level α.

Example: Dimension Reduction



RNA polymerase I = catalyst for protein synthetization (transcription) in eukaryotic ribosomes, from Engel et al. (2013).

- Large biomolecules (DNA, RNA, proteins).

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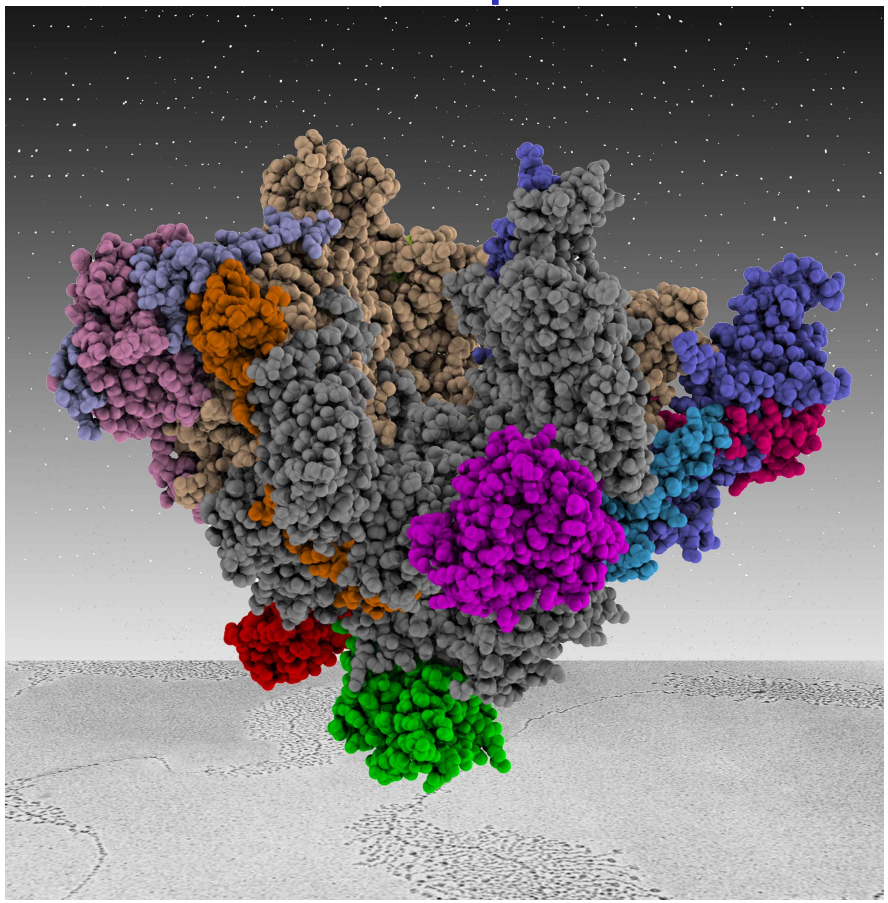

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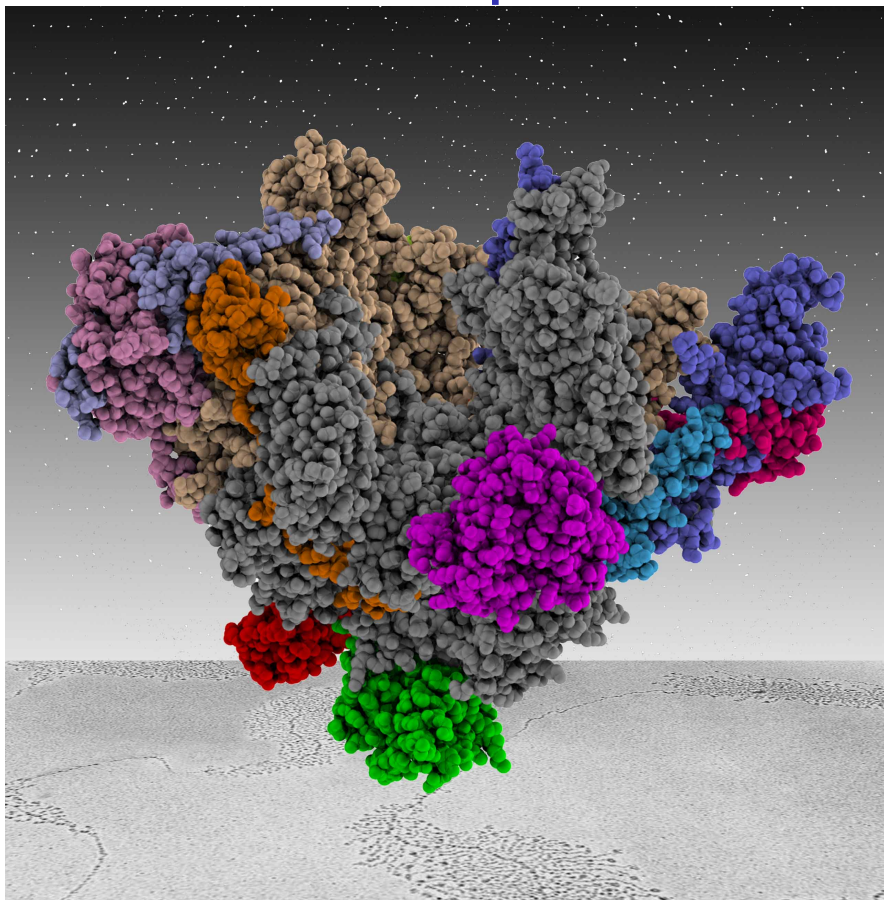

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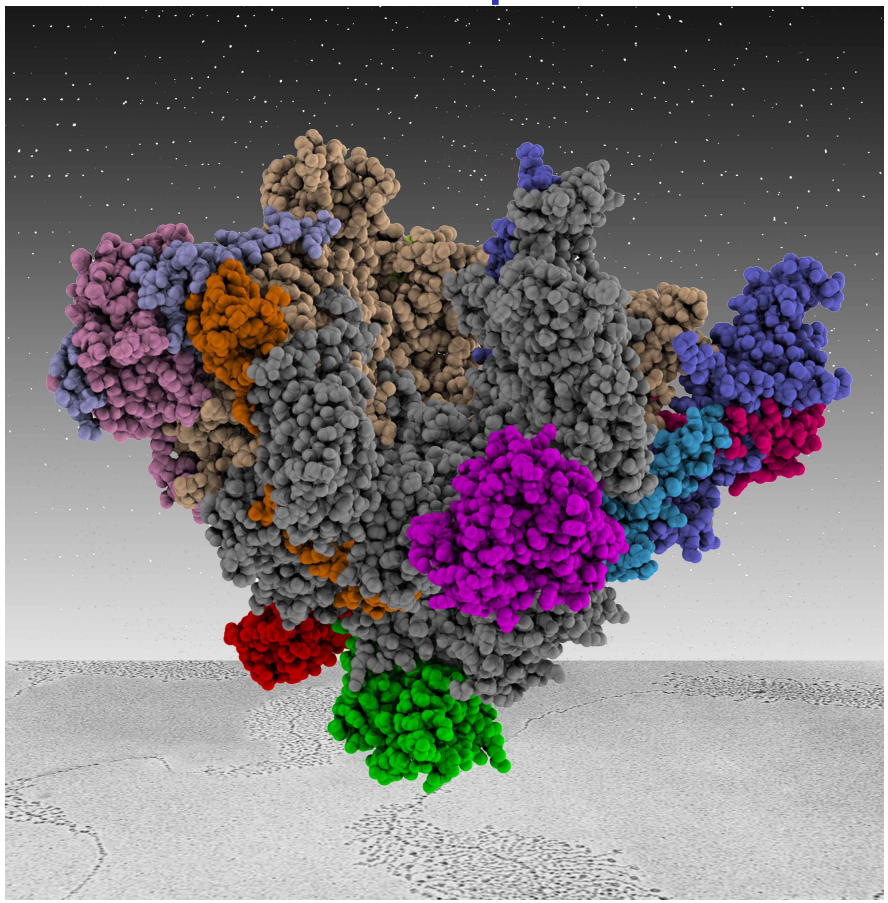

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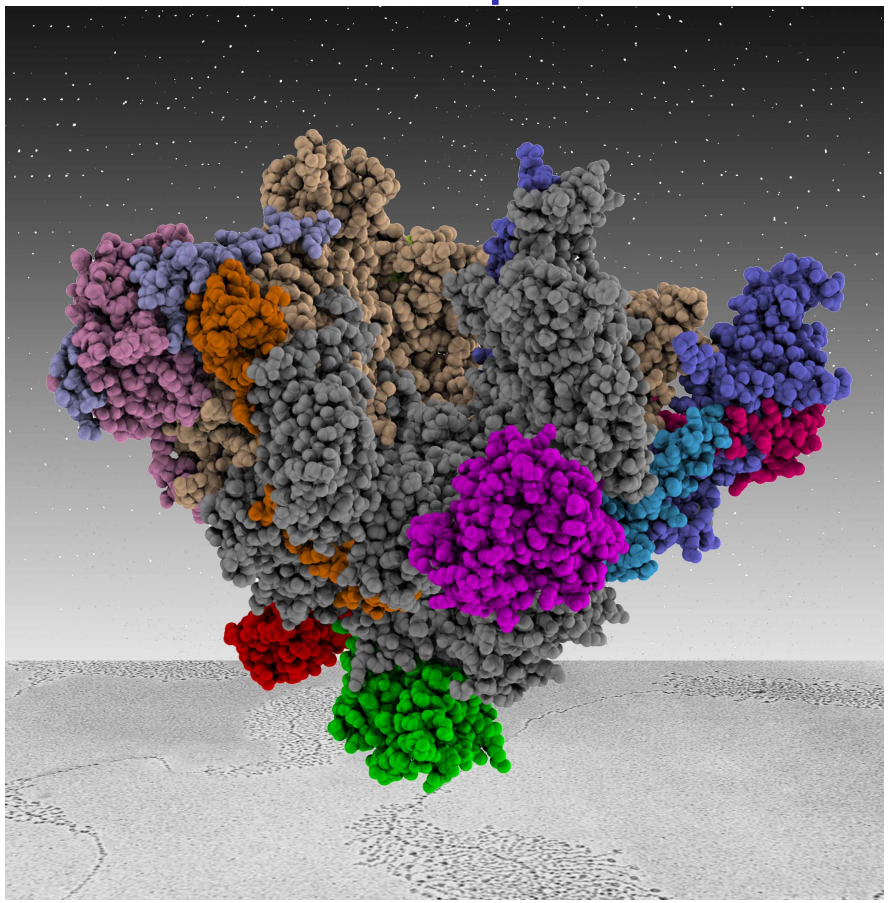

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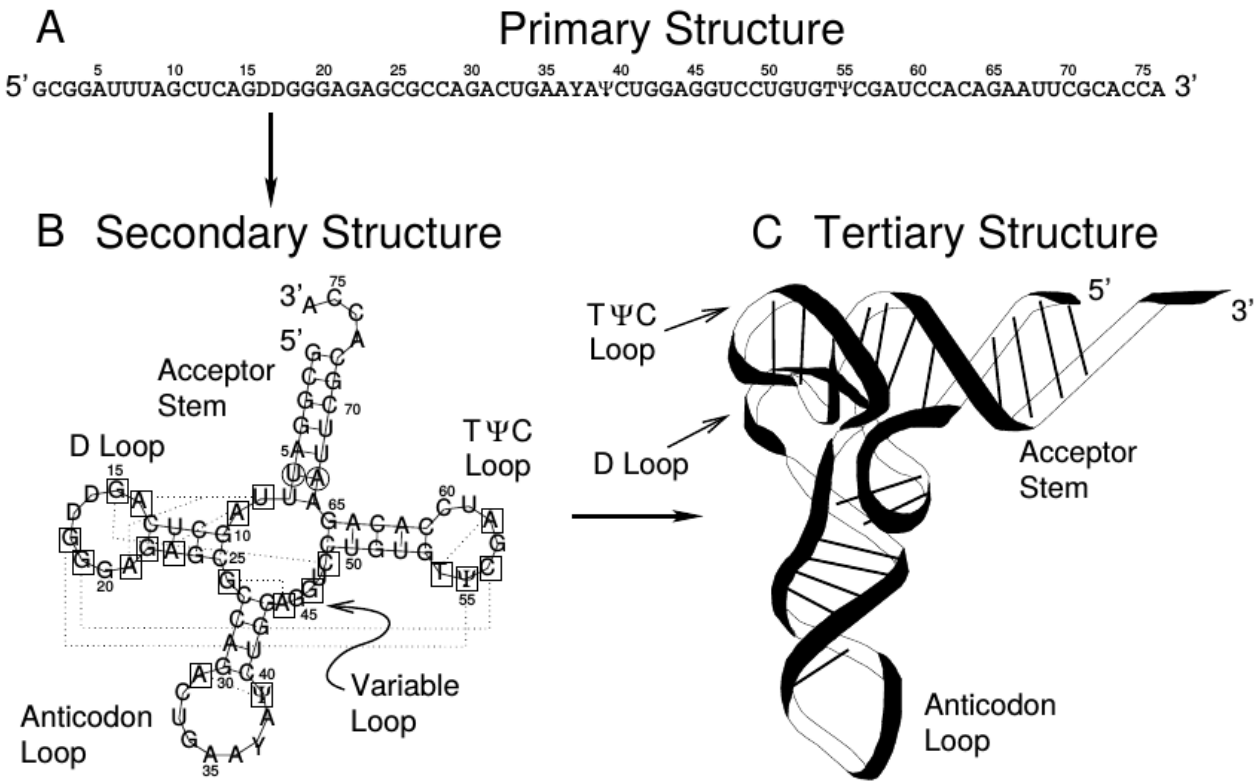
- $\rightarrow$ need for statistical correction and prediction.

tRNA



from Gardner (2003),

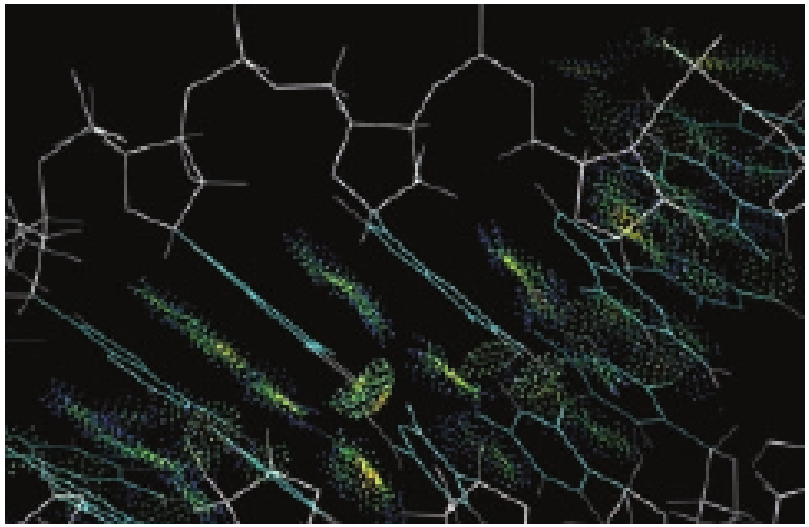
```
# STOCKHOLM 1.0
#=GF ID    trna
#=GF DE    S.cerevisiae tRNA-PHE75 data-set


yeast-PHE1    GCGGAUUUAGCUCAGUUGGGAGAGCGCCAGACUGAAGAUUUGGAGGUCCUGUGUUCGAUC
yeast-PHE2    GCGGAUUUAGCUCAGUUGGGAGAGCGCCAGACUGAAGAUCUGGAGGUCCUGUGUUCGAUC
e.coli-PHE    GCGGAUUUAGCUCAGUUGGGAGAGCGCCAGACUGAAUAUCUGGAGGUCCUGUGUUCGAUC
yeast-PHE3    GCGGACUUAGCUCAGUUGGGAGAGCGCCAGACUGAAGAUCUGGAGGUCCUGUGUUCGAUC
N.crassa-PHE GCGGGUUUAGCUCAGUUGGGAGAGCGUCAGACUGAAGAUCUGAAGGUCGUGUGUUCGAUC
L.luteus-PHE GCGGGGAUAGCUCAGUUGGGAGAGCGUCAGACUGAAGAUCUGAAGGUCCCGUGUUCGAUC
H.vulgarePHE GCGGGGAUAGCUCAGUUGGGAGAGCGUCAGACUGAAGAUCUGAAGGUCGCGUGUUCGAUC
```

Assessing 3D Structure

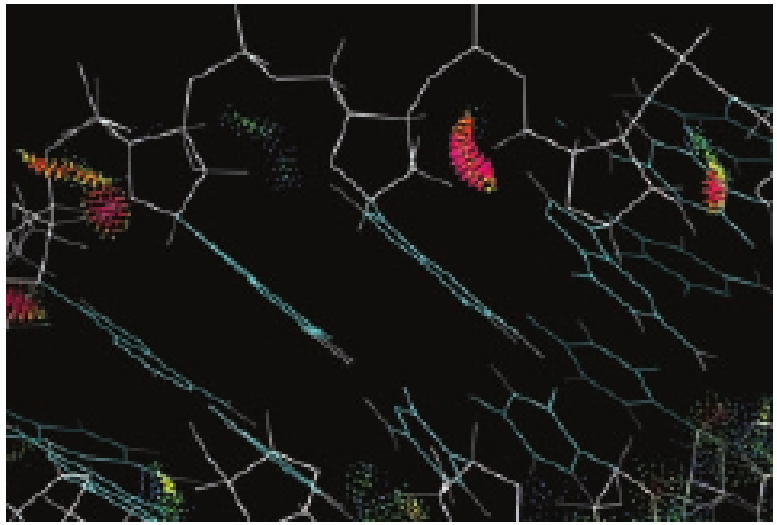
- Build a library linking biological function to geometry.
- Infer biological function of a new unknown primary structure
- by PCA, cf. Frellsen et al. (2009), say.

For ground truth use

- e.g. X-ray crystallography,
- not error free, cf. Murray et al. (2003), often

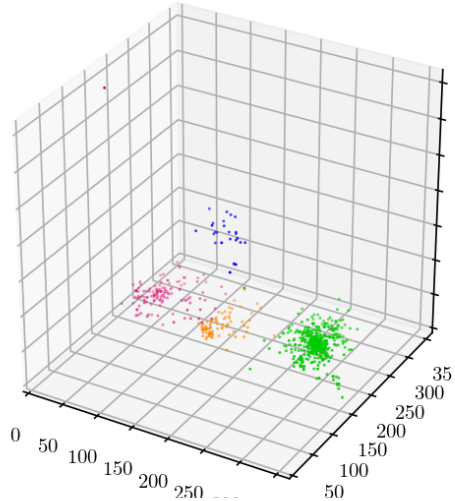


no base clashes

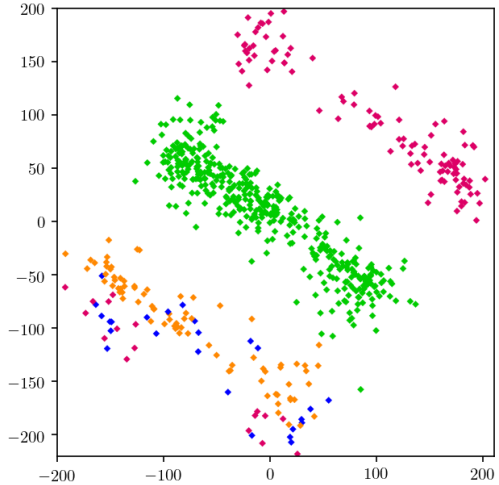


but backbone clashes.

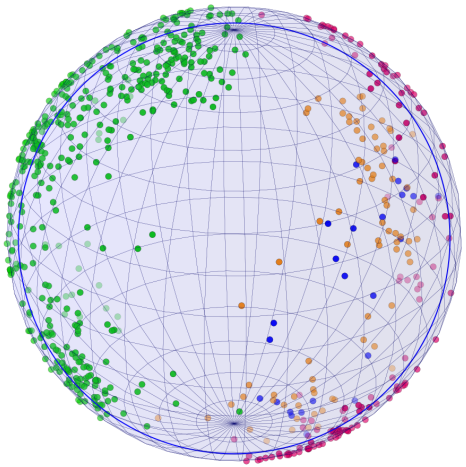
The $C2'$-Endo Sugar Pucker Revisited



3 heminucleotide angles



TS-PCA of 7 angles



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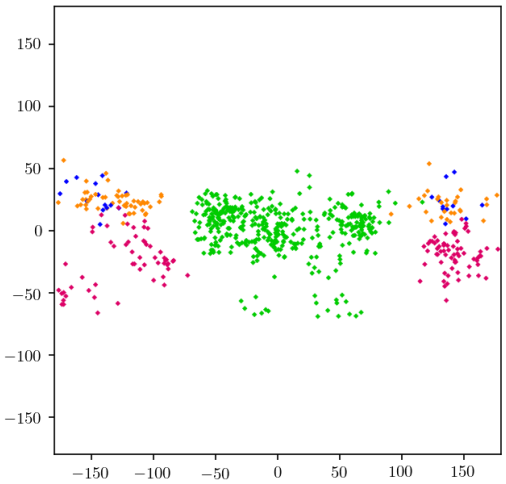
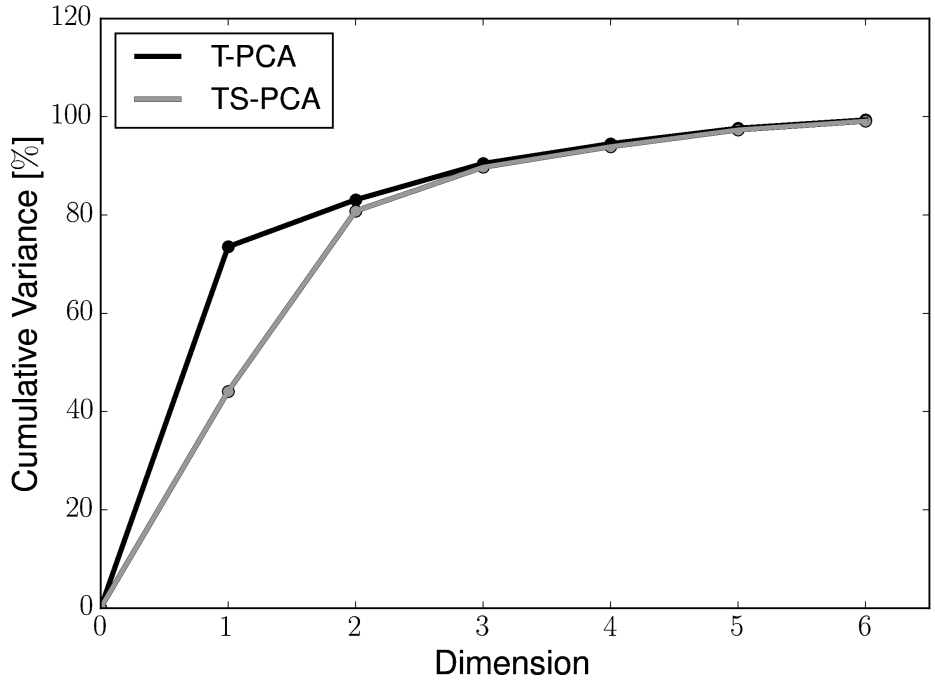


planar view

T-PCA is one dimension ahead of TS-PCA

Indeed, for the $C2'$-endo sugar pucker:



Note that the 2D T-PCA component is almost a great sphere $\Rightarrow$ no subsphere advantage in 2D.

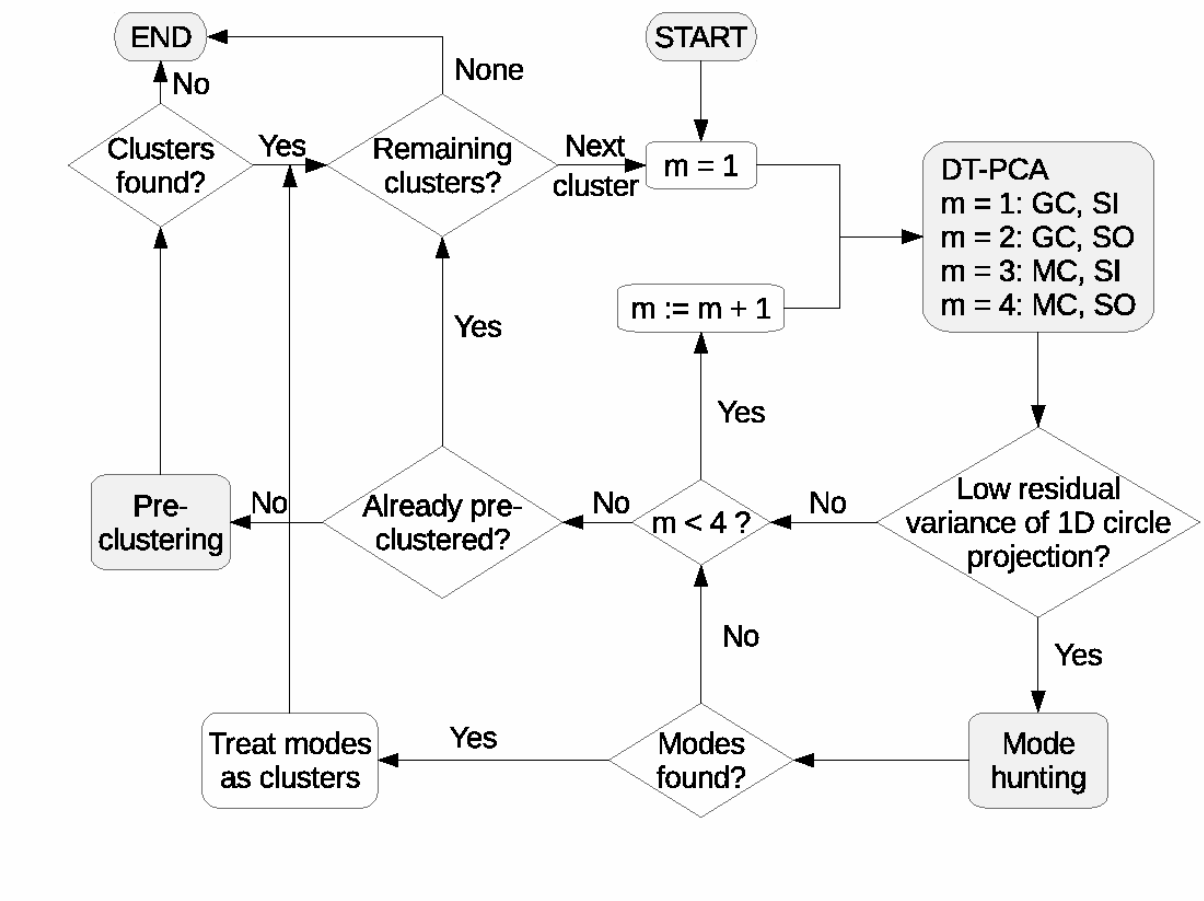
cf. Eltzner et al. (2017).

Clustering to Explore Data Space

- RNA from the RSCB protein data bank
- with high experimental X-ray precision (0.3 nanometers)
- $\rightarrow$ 8301 of 7-angle residues spread out over all of $(\mathbb{S}^1)^7$
- Richardson et al. 2008 perform consensus clustering
- and found 46 clusters: 5 clusters larger than 52 points and 27 below 20 points

	number of points	secondary (sub-)structure
1a (1)	4637	A-form helix
1c (2)	275	"crankshaft version" of 1a
1b (3)	168	leads into 2' suites; k-turn O'
2a (4)	126	leads out of 2' suites; 1-bulge return
1g (5)	78	GNRA1-2; U-turn
	$\vdots$	
1t (45)	7	ttt version of 1b
0i (46)	6	$-\beta$ next to 6n; bases perpendicular

NN Clustering Based on Torus-PCA



Torus-PCA Clustering

We obtain more balanced cluster sizes than Richardson et al. 2008

	number of points	secondary (sub-)structure
1	4921	A-form helix
2	477	interspersed with 1 gives bent/loose helical shapes (“crankshaft version”)
3	232	
4	211	
5	145	
6	139	
7	137	interspersed with 1 give random coils, endings?
	⋮	
22	28	

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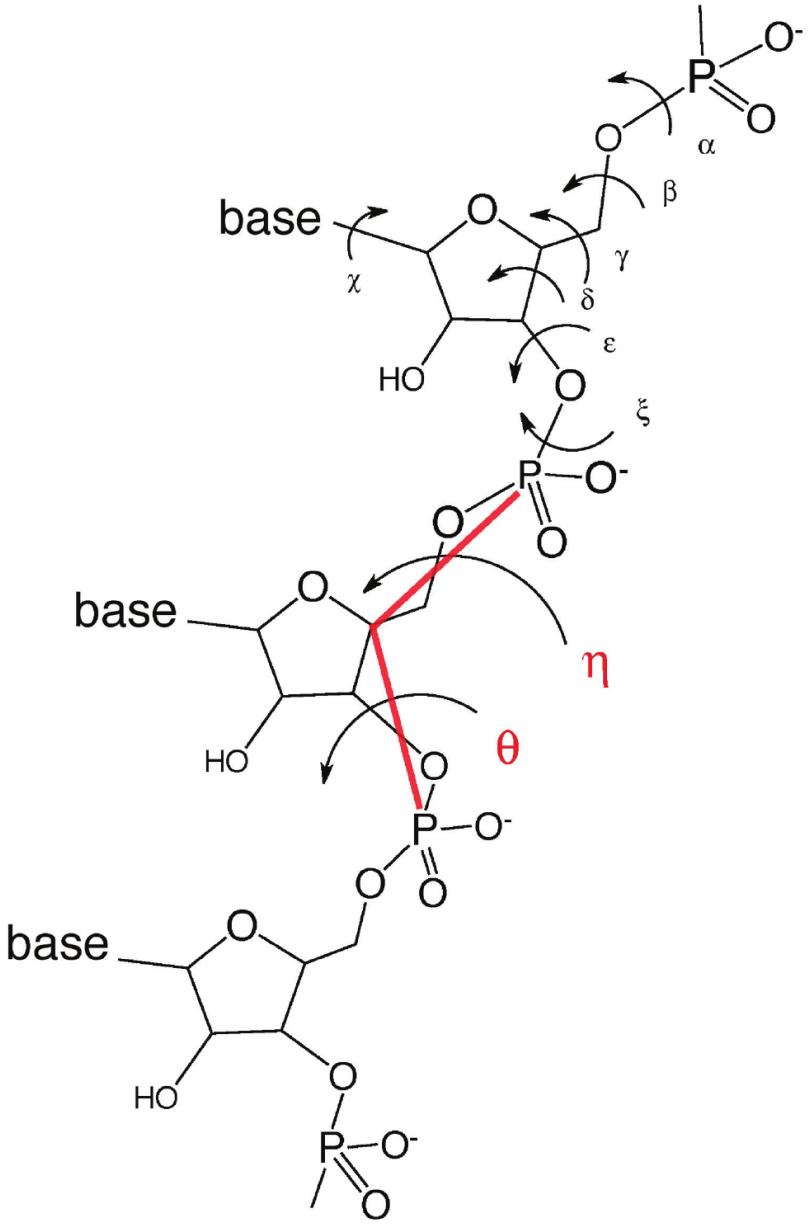
Recall the Dihedral Angles



from Sargsyan et al. (2012)